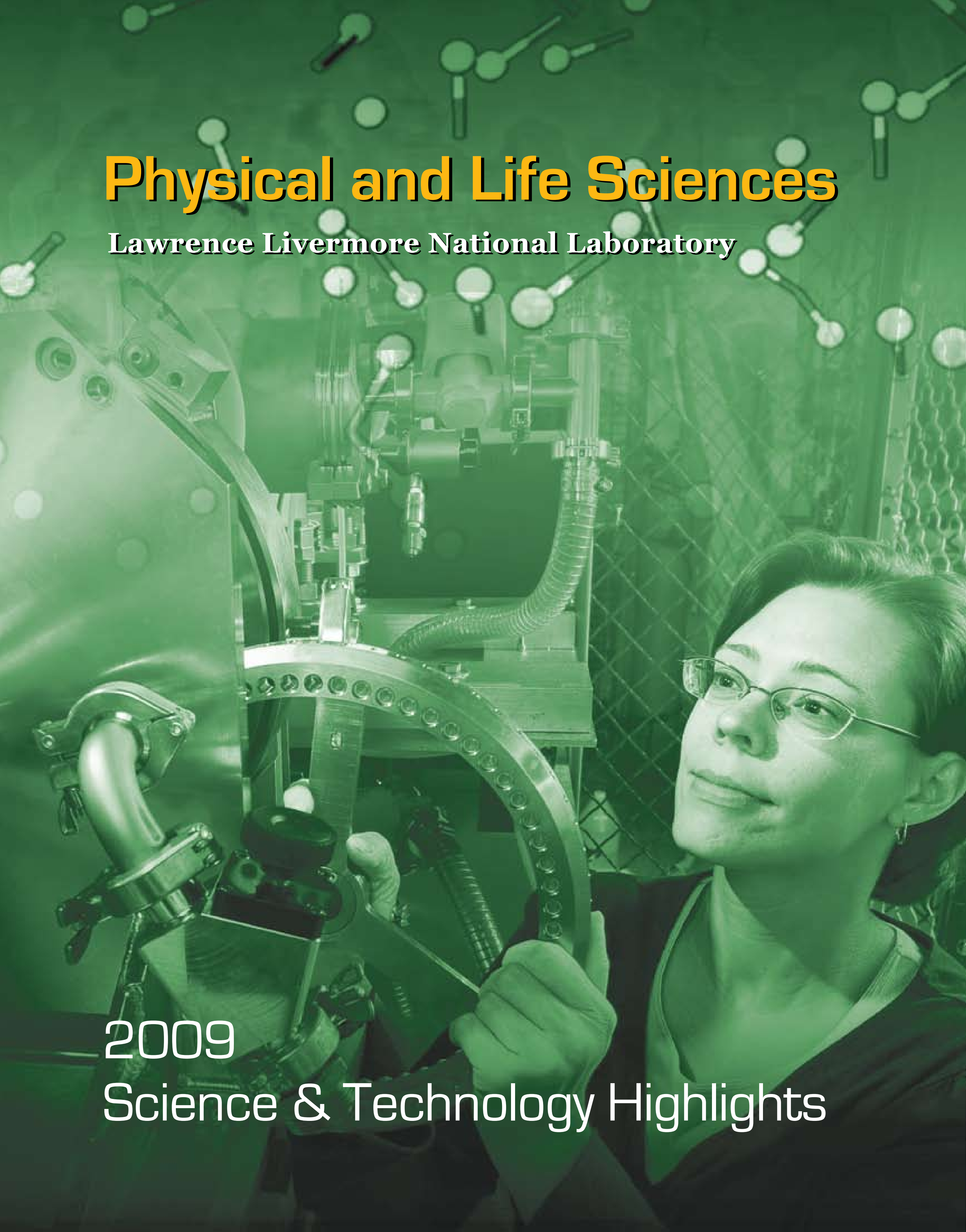
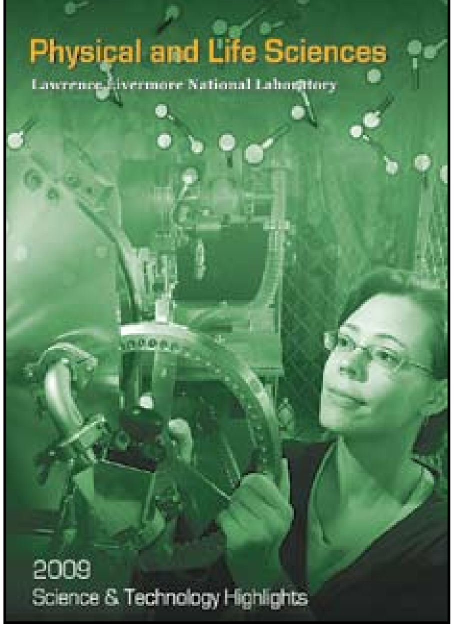
Physical and Life Sciences

Lawrence Livermore National Laboratory



2009
Science & Technology Highlights



About the Cover

A photo of PLS researcher Susan Zimmerman (Atmospheric, Earth and Energy Division) loading a sample wheel into the ion source of the accelerator mass spectrometer at the PLS Center for Accelerator Mass Spectrometry (see "Investigating California's climate record," on page 44) is shown against a background of scientific images from other recent achievements in the PLS Directorate. This collage encapsulates the breadth of science disciplines in PLS—physics, chemistry, materials sciences, earth sciences, and life sciences. This broad range of science enables PLS to achieve its mission of creating and applying knowledge that advances the security and well-being of the nation.

About this Report

This document highlights the outstanding research and development activities in the Physical and Life Sciences Directorate that made news in 2009.

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Don Correll

Publications Editor
Paul Kotta

Designer
Kathy McCullough

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Valuing integrity, innovation, and impact

Message from the Associate Director

"The Physical and Life Sciences mission is to create and apply knowledge that advances the security and well-being of the nation."

William H. Goldstein, PLS Associate Director

The people of LLNL's Physical and Life Sciences Directorate—680 researchers, 80 postdoctoral researchers, 65 student interns, 65 technical support staff, and 60 administrative staff—provide the frontier science and state-of-the-art capabilities needed to solve our nation's hardest problems. This publication represents their work and achievements over the course of 2009.

In these pages you will find stories of scientific discovery, such as the new phase of tantalum hidden between its solid and liquid states; of technological advance, such as a new imaging technique that identifies the microbes that perform specific metabolic tasks within a community; and of impact on problems of national importance, such as a new high-resolution x-ray scanner that keeps an eye on aging nuclear weapon components. The common thread throughout is innovation with impact.

The section "People in the News" highlights the recognition bestowed on our staff for their contributions to the Laboratory, their fields of research, and the nation. I am particularly proud of the recognition given two of our scientists by the President for their service and accomplishments, and by the selection by the American Association for the Advancement of Science of work in PLS as the year's outstanding paper in *Science*. Also noteworthy are the many group and team awards that include members from other LLNL organizations and outside collaborators.

The expertise represented here, ranging from atomic physics to biology, from climate change to nuclear tests, is executed in five divisions:

Atmospheric, Earth and Energy Division (AEED). Supports the Laboratory's defense, global security, and fundamental science programs by conducting research and development (R&D) in the disciplines of atmospheric, earth, and energy science.

Biosciences and Biotechnology Division (BBTD). Performs research in genome biology, computational biology, molecular toxicology, biochemical structures, assays, genetics, microbial biology and pathology, environmental biology, and medical technology.

Chemical Sciences Division (CSD). Executes R&D at the intersections of chemical and nuclear science in support of LLNL's national security missions.

Condensed Matter and Materials Division (CMMD). Maintains integrated and comprehensive condensed matter physics and materials science core competencies for LLNL.

Physics Division. Conducts frontier physics R&D in fields ranging from astrophysics and planetary science, to atomic, nuclear and particle physics, and plasma and high-energy-density physics.

Facilities and Centers. The Directorate operates the Jupiter Laser Facility for high energy density science, the Center for Accelerator Mass Spectrometry, the Glenn T. Seaborg Institute, the Institute for Laser Science Applications, and the Institute for Geophysics and Planetary Physics.

In 2009, PLS research staff authored or co-authored 800 refereed journal articles, filed 80 records of invention and copyrights, and were issued 38 patents. The people of PLS participate in nearly every aspect of the Laboratory's technical work, and as they do, it is with professional and operational integrity foremost.

Directorate Overview

In 2009, researchers within the Physical and Life Sciences (PLS) Directorate continued to make major contributions in support of the missions of Lawrence Livermore National Laboratory in global security, stockpile stewardship, National Ignition Facility science and technology, and fundamental science.

The *PLS 2009 Science and Technology (S&T) Highlights* summarizes the directorate's research and development accomplishments within three sections:

Research in the News, which highlights S&T research accomplishments in the five PLS disciplines.

People in the News, which highlights the recognition of PLS researchers, including scientific awards and fellowships.

Announcements in the News, which highlights external recognition of contributions in addition to research and people.

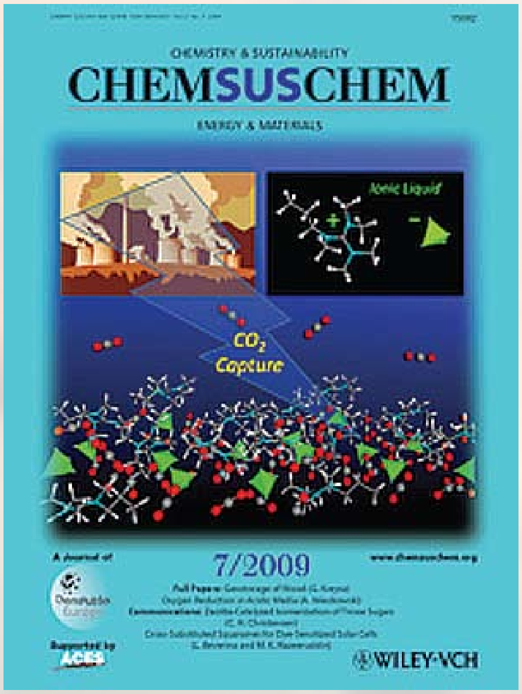
As in previous years, the highlighted accomplishments and recognition are the result of team efforts with other LLNL programs and disciplines, as well as partnerships with other laboratories, industry, and research universities.

PLS enables the Laboratory to accomplish its primary objectives through excellence in the physical and life sciences disciplines. Examples of the 2009 highlights by discipline follow.

Physics Highlight

Beginning on page 8, a Physics highlight describes a new computed tomography scanner device that will enhance NNSA's surveillance program by providing a precise non-destructive means for the detection of aging phenomena on nuclear weapon components for evaluation of potential impact, and to provide a basis for assuring a high level of confidence in their continued performance. Called CoLOSSIS (Confined Large Optical Scintillator Screen and Imaging System), this new high-resolution imaging system is used to scan weapons components to identify any anomalies that require additional attention. The system's software assembles the collected digital radiographs into a large 3-D image that scientists can analyze to discover any problems or anomalies. After nearly a decade of designing and testing at LLNL, the CoLOSSIS installation and qualification was completed in September 2009 at Pantex.

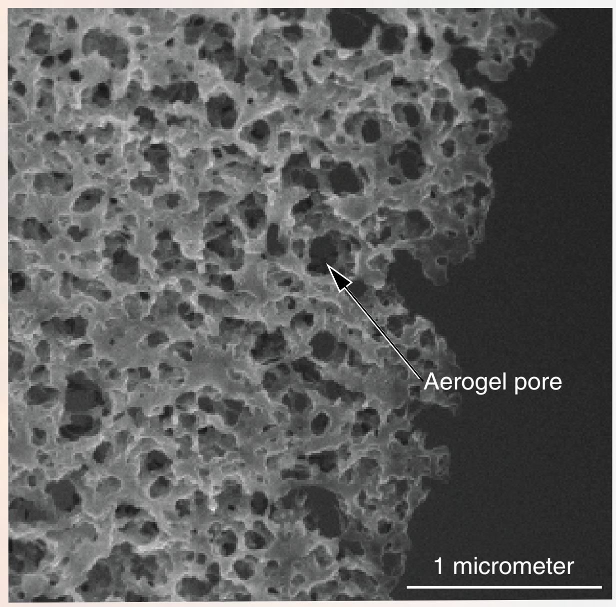
Chemistry Highlight



Beginning on page 18, a Chemistry highlight describes separating carbon dioxide (CO_2) from its polluting source, such as the flue gas from a coal-fired power plant, may soon become cleaner and more efficient. A screening method was developed that would use ionic liquids—a special type of molten salt that becomes liquid under the boiling point of water—to separate carbon dioxide from its source, making it a cleaner, more viable and stable method than what is currently available. Currently, the few coal plants with commercial CO_2 capture capability all use processes based on chemical absorption with monoethanolamine, which unfortunately is nonselective, corrosive, requires the use of large equipment, and effective only under low to moderate partial pressures of CO_2. But the new system overcomes many of these shortcomings.

Material Sciences Highlight

Beginning on page 26, a Materials Sciences highlight describes how aerogels have become exceedingly useful at the Laboratory in laser target fabrication, energetic composites, sensors, ceramics, and coatings. Doping is used to impart additional chemical elements into the matrix. However, this doping process can be challenging because of aerogel's complex pore structure. An efficient method has been developed to dope carbon aerogel with platinum, which is an effective catalyst with many possible applications. Using atomic layer deposition—a gas deposition process that provides atomic-level control of thin films—minute amounts of platinum were added to uniform discs of carbon aerogel.

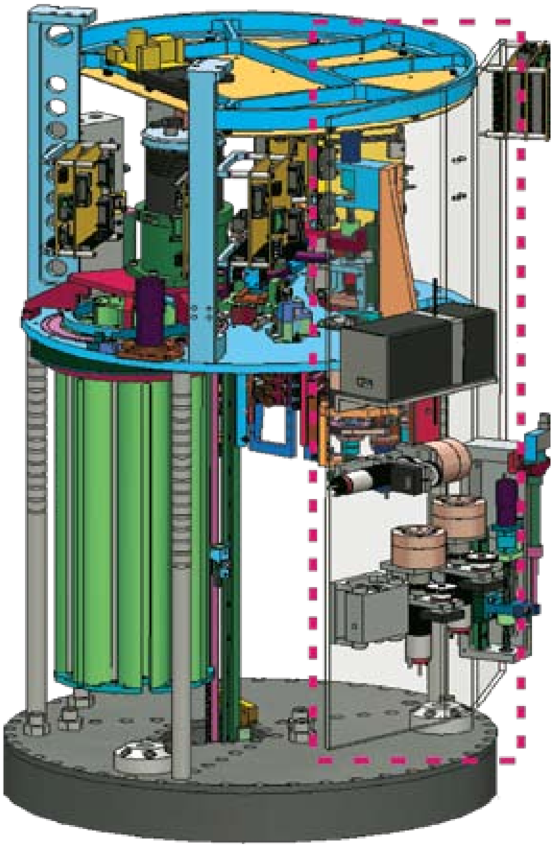


Earth Sciences Highlight

Beginning on page 36, an Earth Sciences highlight describes three proposals accepted by DOE's Office of Energy Efficiency and Renewable Energy under Recovery Act funding for geothermal research. One project will focus on developing realistic computer-based models of enhanced geothermal system (EGS) stimulation-response scenarios. EGS creates an effective subsurface heat exchanger for power generation when the natural system is hot enough but fracture permeability is insufficient. The second project will map microseismicity for geothermal reservoir management to help detect and locate microearthquakes induced by EGS hydrofracturing and fluid reinjection operations in reservoirs. The third project will determine what effect geochemical reactions have on the use of carbon dioxide as an efficient heat exchanger for geothermal energy production.

Life Sciences Highlight

Beginning on page 48, a Life Sciences highlight describes how the search for new life forms has been improved through the use of an autonomous electro-opto-mechanical device that detects microbial genes of interest and measures their preponderance. The device, a polymerase chain reaction (PCR) module, incorporates features from Livermore-designed systems that detect pathogens, but it is much more compact and "intelligent" than previous instruments. Data produced by the PCR module will help researchers better understand the roles microbes may play in responding to global climate change. By studying the genetic makeup of these species, scientists can learn how microbes remove carbon from the atmosphere and cope with the increasing acidity of oceans.



Research in the News

Advancing science and technology in the national interest

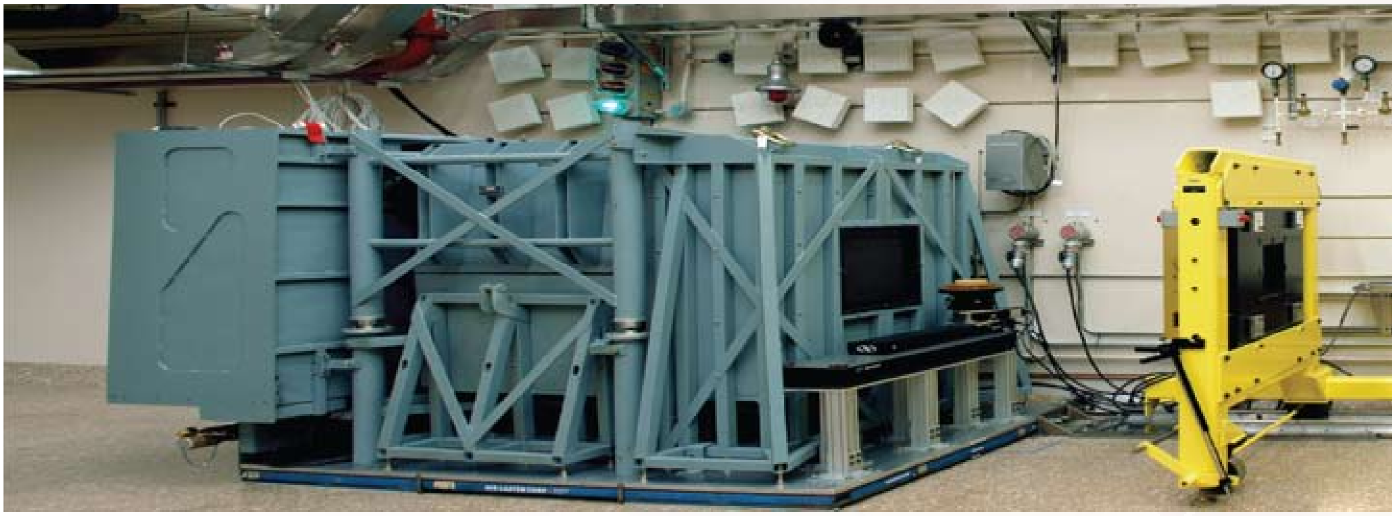
Physics

New scanner inspects weapon components nondestructively

In response to NNSA's need to implement cost effective, optimized inspection of nuclear components (also known as "surveillance transformation"), scientists at Lawrence Livermore National Laboratory (LLNL) teamed with NNSA's Pantex Plant near Amarillo, TX, to develop a new x-ray computed tomography (CT) system to image nuclear weapon components. The new CT scan will enhance NNSA's surveillance program by providing a precise nondestructive means for the detection of aging phenomena on nuclear weapon components for evaluation of potential impact, and to provide a basis for assuring a high level of confidence in their continued performance.

Called CoLOSSIS (Confined Large Optical Scintillator Screen and Imaging System), this new high-resolution imaging system is used to scan weapon components to identify any anomalies that require additional attention. The system's software assembles the collected digital radiographs into a large three-dimensional image that scientists can analyze to discover any problems or anomalies. After nearly a decade of designing and testing at LLNL, the CoLOSSIS installation and qualification was completed in September 2009 at Pantex. The project was managed and supported through NNSA's Enhanced Surveillance and Core Surveillance Programs.

This new capability will be used to detect structural variations arising from so-called "birth defects" or from the aging effects. One key feature of this state-of-the-art, nondestructive tool lies in the fact that it conserves valuable resources and assets by eliminating some destructive procedures and disassembly operations. Future inspections at Pantex will generate detailed, high fidelity surveillance data for scientists at LLNL and Los Alamos National Laboratory. This tool and the associated data that it generates represent a substantial improvement to NNSA's approach to conducting surveillance. Pat Allen, deputy program manager of the Laboratory's enhanced surveillance effort, says, "Without x-ray diagnostic tests at Pantex, we would have to resort to destructive evaluation of these very expensive weapon components. With the right diagnostic tools, we can conserve valuable resources by eliminating some destructive procedures and disassembly operations." Individuals with key roles in CoLOSSIS were Gary Stone (of Physics, who



X rays from a 9-megaelectronvolt (MeV) linear accelerator (far right) travel through three tungsten collimators to the heavily shielded Confined Large Optical Scintillator Screen and Imaging System (CoLOSSIS).

carried out deployment) and Dan Schneberk (of the Computation Directorate, who developed the control and analysis software).

LLNL became the first user of the CoLOSSIS system in support of core surveillance of weapons. LANL will be next to use it, in support of pit surveillance activities for the Air Force's B61 gravity bomb. Inspectors at LANL will assess these components for aging and manufacturing or other defects, and will be provided with never-before-seen three-dimensional characterizations of the components. Scientists will use the valuable data to develop surveillance assessments that could be used in future Life Extension Programs.

"This new system is a prime example of NNSA's ability to leverage the best science and technology in the world to solve complex national security challenges and highlights our commitment to transforming a Cold War nuclear weapons complex into a 21st century nuclear security enterprise," said NNSA Administrator Thomas P. D'Agostino. "We are fortunate to have dedicated scientists working together from across the nuclear security enterprise to develop cutting-edge tools to monitor aging in critical weapon components."

Contact: Gary Stone (925) 423-0987 (stone4@llnl.gov)

Groundbreaking measurements of liquid deuterium compressibility

Damien Hicks, along with his Physics Division colleagues and University of Rochester (UOR) collaborators, has published new, precise measurements of deuterium compressibility under laser-driven shock compression in the January 26, 2009 issue of ***Physical Review B***. Single-shock compressibility of liquid deuterium around 100 GPa has been a source of great theoretical and experimental controversy for over a decade. The measurements by Damien and team, performed at UOR's Omega laser facility, show that deuterium exhibits just over four-fold compression up to 100 GPa, in agreement with published pulsed-power and explosively driven measurements but in disagreement with the laser-driven measurements performed on the Nova laser facility. The LLNL–UOR results resolve a long-standing discrepancy and intriguingly reveal an unpredicted feature in the deuterium Hugoniot at even higher pressures—an abrupt increase in shock density at 110 GPa, giving rise to an up-to-five-fold compression between 110 and 220 GPa. This feature is seen in both single- and double-shock data and shows how the behavior of hydrogen at high pressure continues to yield surprises.

Contact: Damien Hicks (925) 424-5220 (hicks13@llnl.gov)

Scientists coauthor axion coupling article

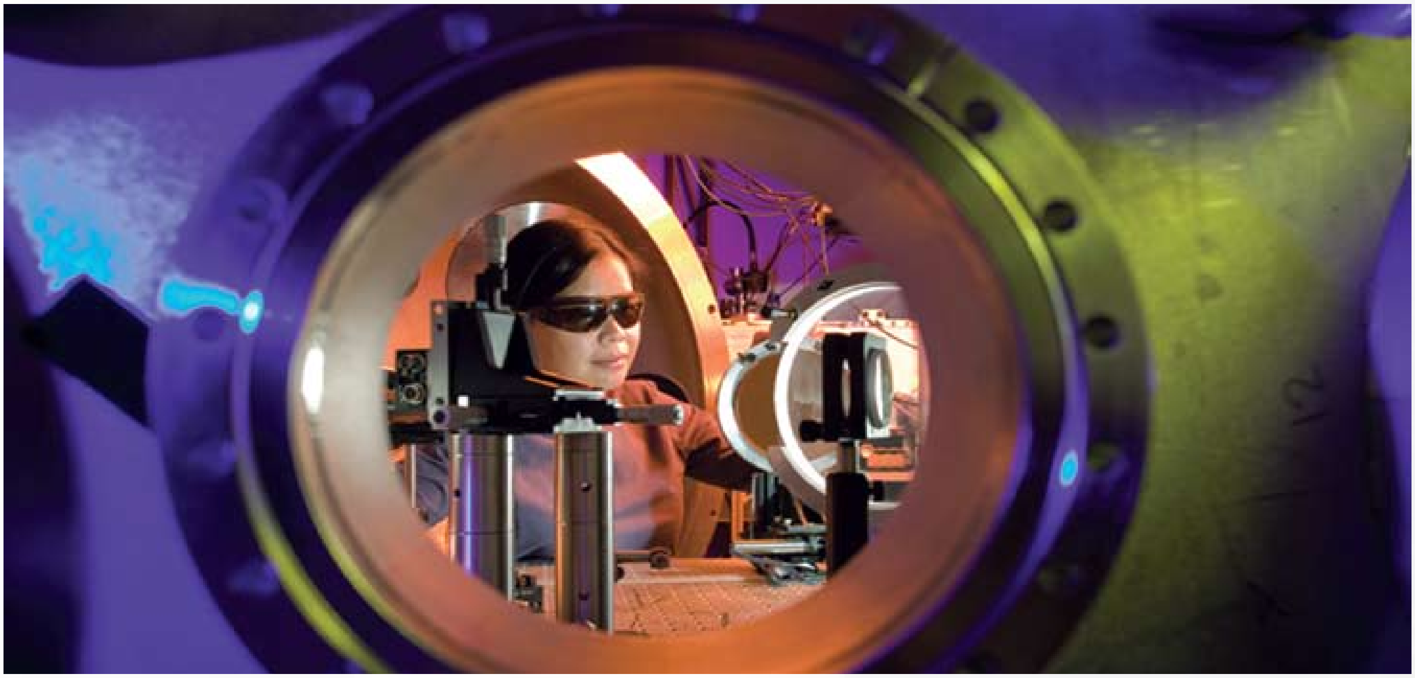
Michael Pivovaroff, Regina Soufli, and Karl van Bibber, of the Physics Division, were coauthors of a ***Journal of Cosmology and Astroparticle Physics*** paper (February 2009 edition) that presents new upper limits on the axion coupling constant determined with the CERN Axion Solar Telescope (CAST). The excluded parameter range covers realistic axion models with a Peccei-Quinn scale (axion decay constant) of approximately 107 GeV. This is the first time laboratory measurements have obtained the sensitivity to exclude theoretical models with axion masses of ~0.1 eV. The article was also the first publication with LLNL coauthors on new CAST results.

Contact: Michael Pivovaroff (925) 422-7779 (pivovaroff1@llnl.gov)

New method yields positrons at greater densities and faster rates than ever before

Researchers at Livermore recently showed that targets thicker than a few micrometers are a more efficient mechanism for positron generation. Using an ultraintense, short-pulse laser and millimeter-thick targets, physicists Hui Chen and Scott Wilks have investigated an improved method for positron generation that has the potential to advance antimatter research. Studying the gamma rays produced when positrons and electrons annihilate each other may help researchers better understand gamma-ray bursts that occur in space. In addition, the method could be used to generate a high-yielding positron source for particle accelerators. The method could also provide a more efficient way to generate positronium gas. Current production methods require positronium gas to be contained in magnetic traps that must be filled repeatedly to obtain the amount needed for research purposes. “Instead of producing positronium gas in small increments over time, we can in principle produce the amount needed for research in a few picoseconds,” says Chen. “The results of this experiment are so new, we have not even begun to investigate all the potential applications,” says Wilks.

The results of this work were published on March 11, 2009 in ***Physical Review Letters***—in which they were featured as one of the journal’s “focus” stories—and were also highlighted in the May 2009 edition of ***Nature Photonics***.



Physicist Hui Chen conducts positron experiments on Livermore’s Titan laser, which couples a high-energy, petawatt short-pulse beam with a kilojoule long-pulse beam.

Contacts: Hui Chen (925)-423-5974 (chen33@llnl.gov) and Scott Wilks (925) 422-2974 (wilks1@llnl.gov)

LLNL collaboration on galaxy evolution featured in *Nature*

PLS Institute for Geophysics and Planetary Physics collaborator Adam Stanford (of UC Davis) and his colleagues from around the world have developed a new picture of galaxy assembly in which bright cluster galaxies experience an early period of rapid growth rather than a prolonged hierarchical assembly. The group first studied the ages of the stars within these galaxies by looking at the infrared wavebands, which, being less sensitive than optical light to the presence of young stars, are a more accurate tracer of the underlying old stellar population and, in turn, of the stellar mass of the systems. The research appeared in the April 2 edition of ***Nature***.

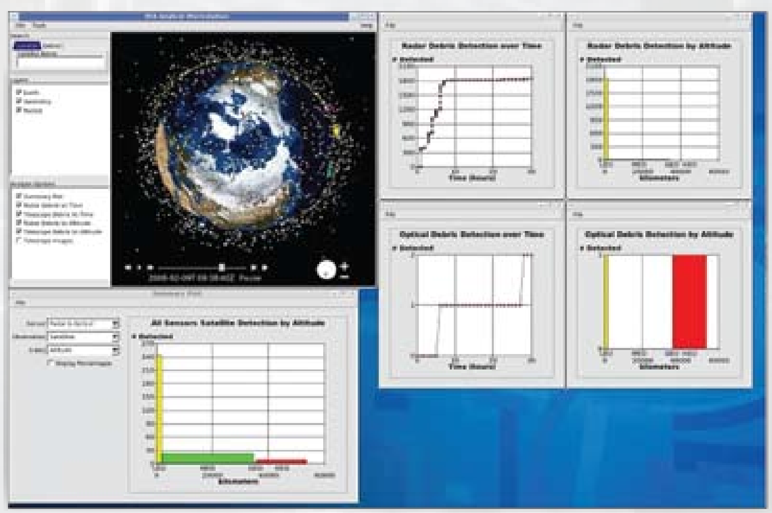
Contact: Adam Stanford (925) 423-6013 (stanford3@llnl.gov)

Designing tools to prevent collisions in space

Orbiting satellites collect and relay vast amounts of data critically needed for civil, commercial, scientific, and national security applications. The U.S. and many other countries depend on space-based systems to navigate, communicate, monitor environmental changes, and provide surveillance data. Lawrence Livermore, in collaboration with Los Alamos and Sandia National Laboratories and the Air Force Research Laboratory, is working to improve capabilities for detecting and monitoring space debris and other threats to space operations. Since 2008, a team of computational physics and engineering experts at LLNL has been designing a comprehensive set of analysis, modeling, simulation, and visualization tools that together are called the Testbed Environment for Space Situational Awareness (TESSA). Physicist Scot Olivier leads the TESSA effort.

With TESSA, the Laboratory is improving the capability to analyze the performance of the collection of radio-frequency and optical sensing systems, called the Space Surveillance Network (SSN), currently used by U.S. Air Force Space Command to monitor activities in space. TESSA can also be used to assess the relative efficacy of new sensor configurations and operational methods. TESSA exploits the Laboratory's expertise in high-performance computing, optical and radio-frequency phenomenology and instrumentation, the physics of hypervelocity impacts, and data mining, a statistical process that quickly sifts through mountains of information to locate the important nuggets.

The urgency of the TESSA team's work was underscored by the February 10, 2009 collision between the defunct Russian satellite Cosmos 2251 and the operational communications satellite Iridium 33. "It provided the first opportunity for Livermore to use its modeling tools in a live situation," says physicist Alex Pertica, who is chiefly responsible for project execution. Working closely with U.S. Air Force Space Command, the LLNL team used Livermore's explicit hydrodynamics code ParaDyn to perform detailed, high-performance computer simulations of the expected distribution of debris from the collision, then computed the increased risk to other satellites posed by this new debris in order to determine whether this risk was high enough to justify repositioning specific assets. The conclusion—the collision risk for over a hundred active satellites was increased by about 50%—was not enough to warrant disrupting operations to



The TESSA User-Defined Operational Picture is a customizable environment for visualizing orbiting objects and the results of simulations. This graphical user interface is available on the desktop of all TESSA users.

reposition any specific systems, but did highlight a worrying trend—with every collision, the resulting debris increases the risk of future collisions.

TESSA initially focused its efforts on debris simulations. "Now, the scope is much broader," says Scot. "We are modeling space operations in a unified framework and moving from surveillance to a broader awareness of what is occurring in space. We need the capability to quickly and accurately predict an event, such as a collision, before it occurs." The U.S. Air Force Space Command and the National Reconnaissance Office have joined to create a new national program to coordinate space-protection activities across the military and intelligence communities. TESSA is now being used to support these activities and could eventually be fully integrated into the U.S. Air Force Joint Space Operations Center.

Contacts: Scot Olivier (925) 423-6483 (olivier1@llnl.gov) and Alex Pertica (925) 423-3354 (pertica1@llnl.gov)

Paper selected by *Physical Review B* as Editors' Suggestion

Michael Manley, with colleagues from Cornell University, the National Institute of Standards and Technology, the University of Maryland, and Los Alamos and Argonne National Laboratories, successfully showed that under certain equilibrium conditions, energy in a crystal is not distributed uniformly but is, in fact, concentrated in small regions randomly throughout the crystal. The possibility of such dynamic nonlinear hot spots—also known as intrinsic localized modes—has been understood theoretically for more than 20 years but rarely observed. The paper describing these results appeared in the April 22, 2009 edition of ***Physical Review B*** and was also selected as an Editors' Suggestion.

Contact: Michael Manley (925) 424-6927 (manley3@llnl.gov)

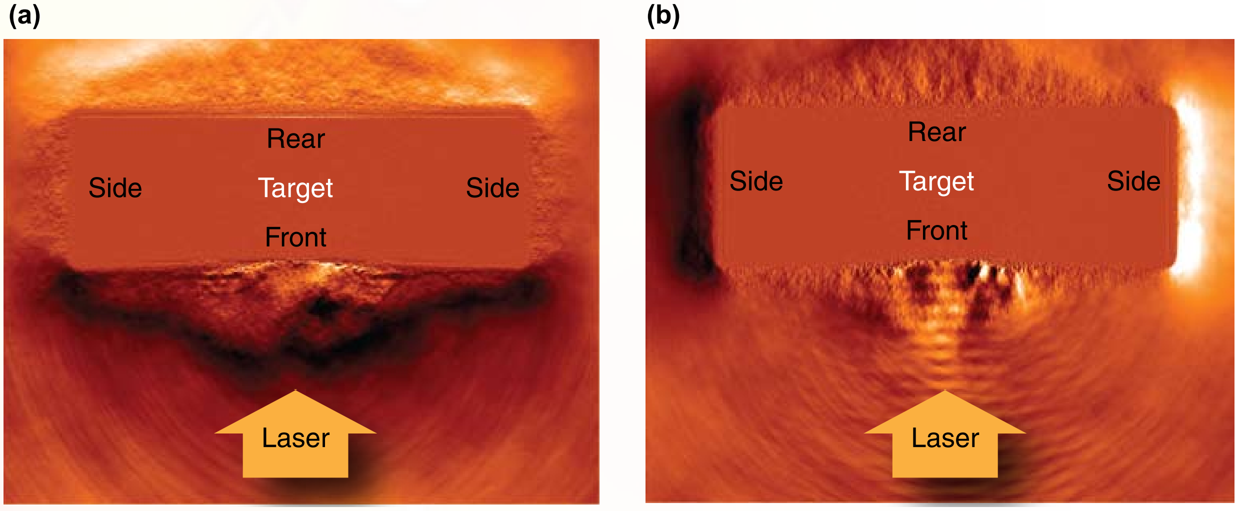
Collaboration using LLNL's BlueGene/L leads to "quantum" leap

Ron Soltz, Pavlos Vranas, Tom Luu, Michael Cheng, and others, working with colleagues at LANL, BNL, Columbia, and the University of Utah, have extended their calculations to understand changes of state that occur when, according to the theory of quantum chromodynamics (QCD), the quarks that make up the protons and neutrons in normal nuclear matter become deconfined in a quark-gluon plasma when heated or compressed. The equation of state is used in a hydrodynamic model for heavy ion collisions at the Relativistic Heavy Ion Collider. The research, published in the July 1, 2009 edition of ***Physical Review D***, is of special interest to the Office of Science in the areas of nuclear and high-energy physics. Early stages of this research contributed to a Gordon Bell Special Achievement Prize in 2006, a contest-winning essay ("Simulating the Birth of the Universe on Petaflop") in the November 2007 issue of ***CISE***, and a new QCD effort at LLNL to calculate the nucleon–nucleon potential and physics beyond the Standard Model that may be observed at the Large Hadron Collider.

Contact: Ron Soltz (925) 423-2647 (soltz1@llnl.gov)

Simulations corroborate high-energy-density experiments

Recently, a Computing Grand Challenge project on Livermore's Atlas supercomputer simulated the results from two sets of laser-driven high-energy-density (HED) experiments. These simulations have helped explain the physics behind what was seen and measured in the experiments. Simulating the physics of the experiments on powerful supercomputers is often the only way to both understand the results in detail and develop physical insight into these complex processes. Simulations can parse the physical constituents that affect the whole and examine microscopic details not easily detected during an experiment. In addition, computer simulations can explore regimes of temperature, density, and pressure that experiments cannot



Two-dimensional simulations help explain the Jupiter Laser Facility Callisto laser experimental results. Electrons accelerated by the laser generate an electric field (a) on both the front and rear of the reduced-mass target and (b) on the target sides.

yet achieve, serving as a guide for future experiments. Ultimately, scientists must depend on both experiments and simulations working in tandem to advance HED physics research.

In one set of HED experiments, researchers used ultrahigh-intensity lasers with ultrashort pulses to zap one side of a reduced-mass target. The small, square targets (100 micrometers across and 7 micrometers thick) were initially designed for studying certain aspects of neutron stars. The goal was to get a dense target as hot as possible in the presence of a large magnetic field. The 2007 experiments performed on the Callisto laser in Livermore's Jupiter Laser Facility showed that the target did get hot, but an unexpectedly large number of protons were ejected from the entire surface of the target. In contrast, when a laser zaps a larger (millimeter size) target, a beamlike pattern of protons blows off the back of the target.

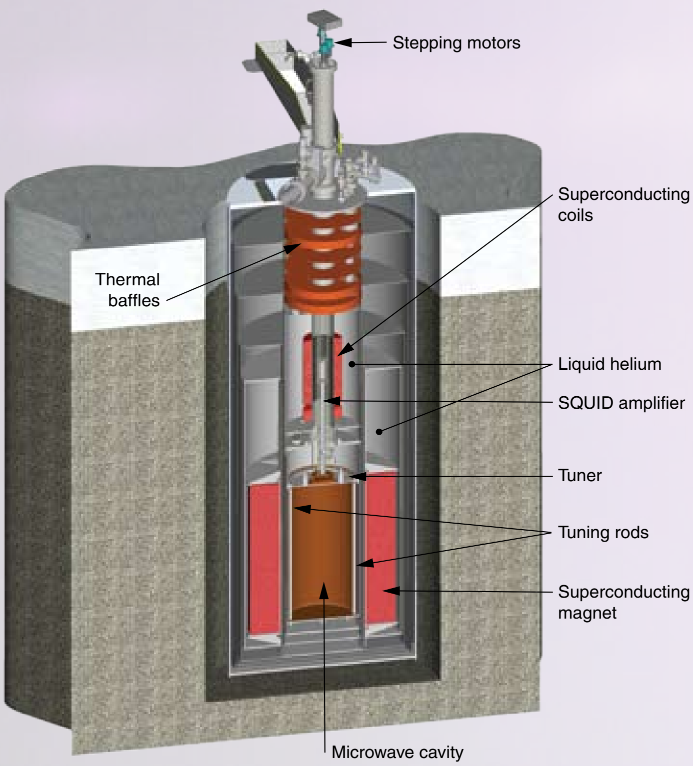
To simulate experimental results, physicist Andreas Kemp used the Particle Simulation Code (PSC), a particle-in-cell code specifically designed for studying electrons in high-energy plasmas. The computational capabilities of Atlas allowed Kemp to simulate laser–plasma interactions in reduced-mass targets at full scale from first principles. In a two-dimensional simulation of a large target, electrons accelerated by the laser generated an electric field on both the top and bottom of the target. In a simulation of a smaller, "finite" reduced-mass target, large electric fields developed on the sides of the target as well, which explained the signal detected all around the target in experiments. This simulation showed that shrinking a target to a smaller size does not increase target temperature but instead increases the total number of ions accelerated from all of its surfaces.

Particle-in-cell simulations of plasma incorporate particles moving in space with an electromagnetic field on a grid. The particles are discrete objects, while the electromagnetic field is continuous. The discrete particles and interpolation from the grid create noise in the simulations. Two-dimensional simulations showed that these new algorithms more accurately model the electron-beam divergence and energy spread measured in earlier experiments. Three-dimensional modeling verified that the algorithms reduce noise and also incorporate more realistic physics. This new accuracy allows design of next-generation experiments to further improve beam quality.

Contacts: Andreas Kemp (925) 423-5941 (kemp7@llnl.gov) and Scott Wilks (925) 422-2974 (wilks1@llnl.gov)

Detectors aid search for dark matter

Many scientists hypothesize that a subatomic particle, called an axion, constitutes dark matter, which is thought to comprise more than 20 percent of the universe. These scientists calculate that every cubic centimeter of space could contain about 100 trillion axions, all produced during the Big Bang some 12 billion years ago. Axions have no electric charge or spin, extremely small mass (a trillion times less than that of an electron), and little interaction with ordinary matter. As a result, detecting these invisible particles requires extremely sensitive equipment. A Livermore experiment, known as the Axion Dark Matter Experiment (ADMX), is designed to find the elusive particle by measuring its decay into a microwave photon in the presence of a strong magnetic field.



A cross section of the ADMX device. Stepper motors move a set of tuning rods in the cylinder's cavity to adjust the cavity's frequency. Helium cools the cavity, reducing the background noise so the ultrasensitive SQUID amplifiers can boost the faint axion signal.

The microwave photon's faint signal must be amplified to an extreme degree to be detected. The capacity to distinguish weak photons during axion decay was significantly enhanced in 2008 when the ADMX team adopted sensitive amplifiers about the size of computer chips—high-gain, ultralow-noise amplifiers are based on superconducting quantum interference devices (SQUIDs). Darin Kinion fabricated the units in cooperation with the University of California at Berkeley.

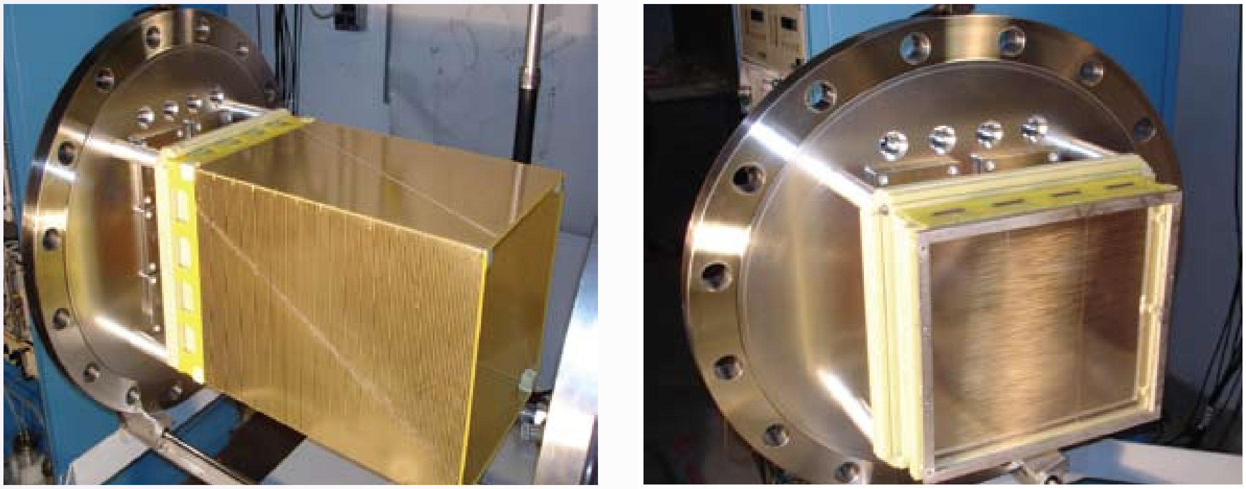
Contact: Darin Kinion (925) 422-8798 (kinion1@llnl.gov).

Detecting illicit nuclear materials from their neutron emissions

A time-projection chamber (TPC) is a gas-filled device that measures charged-particle trajectories in three dimensions. The instruments are used in high-energy physics experiments to track particles after they are "smashed" together inside particle accelerators. In collaboration with other research institutions, a Livermore team led by Physics Division scientist Mike Heffner is creating a robust, field-ready neutron TPC (nTPC) that can be used by nonexperts to locate fissile materials in nonproliferation and nuclear counterterrorism efforts. Using nTPC, personnel could detect the presence of neutrons emitted from a radioactive source within minutes. In addition, the nTPC prototype can indicate the direction of a neutron source from up to 20 meters away.

The nTPC prototype contains hydrogen gas, a lightweight medium that interacts with fast neutrons. When a fast neutron enters the gas, it collides with a hydrogen atom, causing the proton to recoil away at an angle. As the newly liberated proton travels along its path, it ionizes the gas, creating an ionization track. The nTPC detects the electrons from the ionization track to determine the proton's trajectory and ionization energy loss. This data is then used to help determine the incoming neutron's trajectory and energy.

(a) (b)



(a) The neutron time-projection chamber contains hydrogen gas, which is surrounded by a "cage" that produces a uniform electric field. (b) A structure at the ground end of the chamber amplifies the electric charge. This grid is used to record the amplified electric signals and provide a two-dimensional set of coordinates for each cluster of electrons.

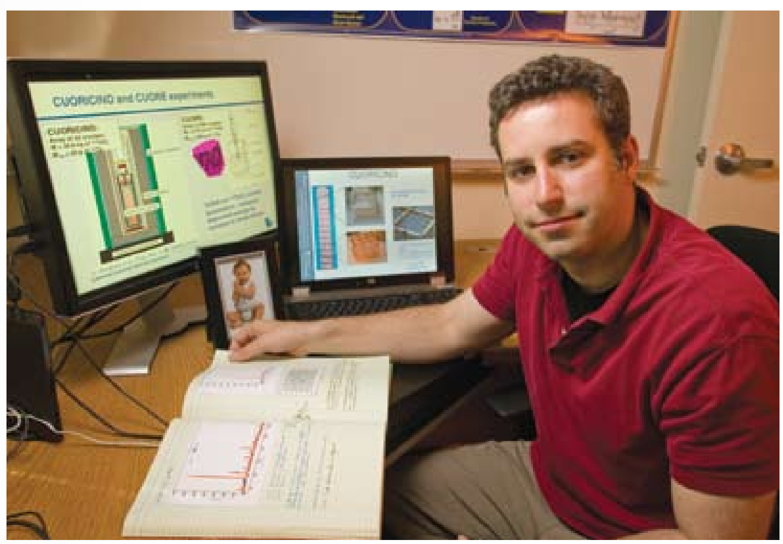
To test the nTPC prototype, Livermore researchers exposed the detector to a californium-252 source equivalent in neutron output to approximately 6 kilograms of weapons-grade plutonium. Inside a laboratory, the team first ran nTPC with the californium source stored in a shielded container to assess the amount of background radiation being generated from neutrons naturally occurring in the environment. The californium-252 source was then removed from the container and placed in various locations several meters from the nTPC. "We detected neutrons from the radioactive source 10 and 20 meters away," says Heffner.

The nTPC has three main advantages. First, the machine provides fast proximity searching because it can "point" in the direction of the sources. Second, it provides improved suppression of background radiation from sources such as cosmic rays and those naturally given off by the decay of isotopes in the environment. Third, nTPC can track multiple neutron sources in the same area.

Contact: Mike Heffner (925) 422-6762 (heffner2@llnl.gov)

Lawrence Fellow hunts for extremely rare phenomenon

Nicholas Scielzo, a postdoctoral researcher who came to Livermore as part of the Lawrence



Lawrence Fellow Nicholas Scielzo is working on an international project to detect a rare radioactive decay process.

Fellowship Program, splits his time between three nuclear physics projects. One involves searching for a long-sought-after radioactive process known as neutrinoless double-beta decay. In this decay, two neutrons in a nucleus are converted to two protons, with the emission of two beta particles, while the accompanying two neutrinos that would normally be emitted in standard double-beta decay annihilate each other instead. "However," says Scielzo, "this decay can only occur if a neutrino and its antimatter partner, the antineutrino, are the same particle." Scielzo is working with U.S. and Italian collaborators to build an extremely sensitive detector to identify this rare decay mode.

CUORE, the Cryogenic Underground Observatory for Rare Events, will be a 1-ton detector located deep underground within Italy's Gran Sasso National Laboratory. The detector will contain an array of nearly 1,000 tellurium dioxide crystals, each a 5-centimeter cube. Tellurium-130 is one of the few isotopes that only decays by double-beta decay and thus could theoretically undergo the neutrinoless process. The crystals will be cooled to 0.01 Kelvin above absolute zero, at which point each crystal's heat capacity is small enough that the energy from a single radioactive decay within the crystal will be detected. As part of his research, Scielzo ensures the crystals meet the team's strict specifications by testing all raw materials used to make the crystals and developing the appropriate crystal growth and surface processing techniques. In addition, to precisely determine where to search for the signal, Scielzo measured the energy released in double-beta decay using a Penning trap mass spectrometer.

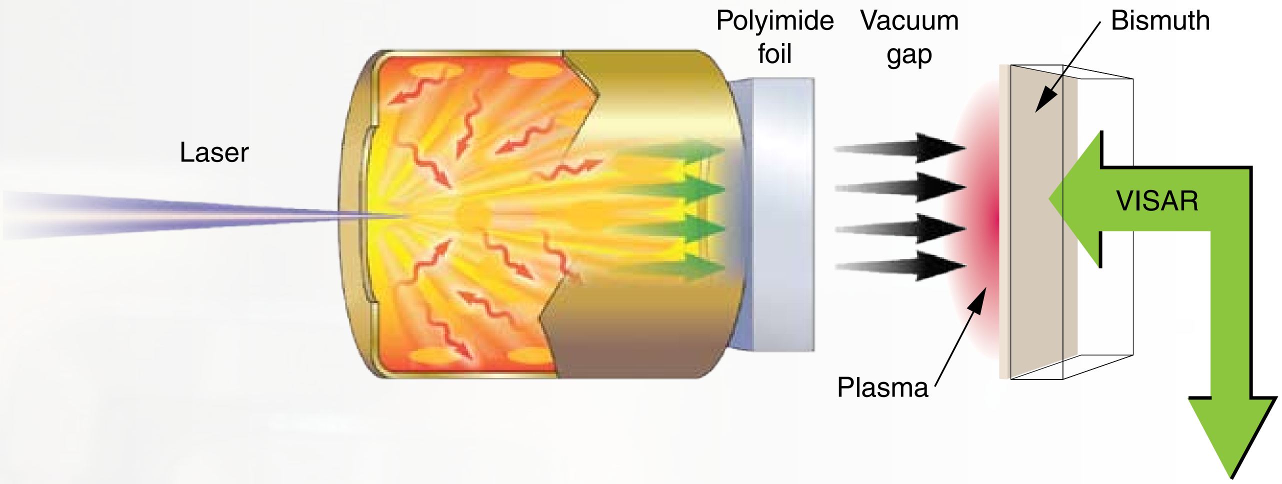
CUORE must collect data for up to 5 years to have the sensitivity needed to make a discovery. However, researchers on the project know that what they may find is well worth the wait. "The CUORE experiment has the potential to reveal interesting properties of neutrinos that no other experiments have been able to show," says Scielzo. In addition to proving that the neutrino and antineutrino are identical, these experiments could help identify the neutrino mass hierarchy and scale and explain why matter dominates over antimatter in the universe. "The experiments won't tell us everything we want to know about the formation of our universe," says Scielzo, "but they could provide one component of the larger explanation."

Contacts: Nicholas Scielzo (925) 422-4172 (scielzo1@llnl.gov)

Laser-driven compression re-creates conditions inside planets

Laser-driven ramp compression can achieve high states of compression in a target material while simultaneously keeping the material relatively cool so scientists can examine the material under high pressures. Under extremely high pressures, the target material may remain in its initial phase, or it may change from a solid to a liquid, or from one solid phase to another. Ramp compression offers the first continuous view of the phase transition and thus will help scientists better understand the physics of solids at extreme conditions. "We now can see how quickly the transition mechanisms happen," says physicist Ray Smith, who leads the ramp-compression research team in PLS.

Because of these unique attributes, ramp compression is the only tool that will allow scientists to examine the interior structure of exoplanets—planets in other solar systems—that are similar to but larger than Earth. Recent discoveries indicate that other solar systems contain a new family of terrestrial planets more massive than Earth but smaller than the gas giants. These so-called super-Earth planets range from 1 to 10 times the mass of Earth, with pressures at their core from 3,000 to 5,000 GPa. Although ramp-compression experiments have yet to achieve the high pressures at a planet's core, they can re-create the phase transitions occurring well beneath an exoplanet's surface. Scientists can thus use this laser method to test various planetary hypotheses, such as whether Uranus has a solid diamond core.



In the ramp-compression experiments, a laser pulse strikes polyimide foil. Polyimide launches across the vacuum gap and hits the bismuth sample, generating a ramp-compression wave. The VISAR (Velocity Interferometer System for Any Reflector) diagnostic records the wave's time history.

Smith's team has developed the techniques and diagnostic tools essential for routine high-pressure ramp-compression experiments. In a typical application, a polyimide foil is targeted with a laser. The pulse strikes and rarefies the foil, launching polyimide across the vacuum gap. This hits the bismuth sample and launches a ramp-compression wave. A diagnostic tool called VISAR (Velocity Interferometer System for Any Reflector) records the time history of the compression wave.

Recent experiments led by physicist Dave Bradley compressed diamond, a solid phase of carbon, using the higher energy Omega laser at the University of Rochester. These experiments yielded the highest ramp-compression pressures ever reported, 1,400 GPa, as well as the highest-pressure solid equation-of-state data. Data for pressure versus density indicate that the diamond phase is stable with significant material strength up to at least 800 GPa. This work appeared in the February 20, 2009 edition of ***Physical Review Letters***.

Contacts: Dave Bradley (925) 424-5837 (bradley9@llnl.gov) and Ray Smith (925) 423-5895 (smith248@llnl.gov)

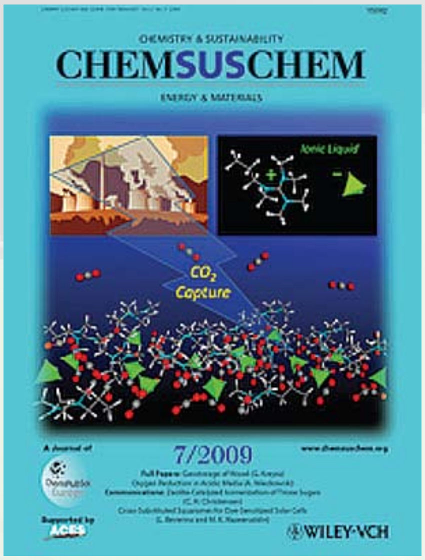
Research published in *Nature Physics*

A paper by Jon Eggert and co-authors Rip Collins, Damien Hicks, Peter Celliers, and David Bradley (all in the Physical Sciences Division) was published online in ***Nature Physics*** on November 8, 2009. The paper—"Melting temperature of diamond at ultrahigh pressure"—describes the melting temperature of diamond, the metallization of shock-compressed diamond, and the polymerization of carbon at pressures up to 20 Mbar. This paper shows the melt curve for diamond is nearly flat to 11 Mbar—ten times higher than any previous melt measurement—and reveals new and unexpected chemistry in the liquid phase of carbon. In short, this paper provides a small window into a very new world of materials science at high-energy-density conditions.

Contact: Jon Eggert (925) 422-3249 (eggert1@llnl.gov)

Chemistry

Cleaner, more efficient method developed to capture CO_2



Separating carbon dioxide (CO_2) from its polluting source, such as the flue gas from a coal-fired power plant, may soon become cleaner and more efficient. A Lawrence Livermore researcher has developed a screening method that would use ionic liquids—a special type of molten salt that becomes liquid under the boiling point of water—to separate carbon dioxide from its source, making it a cleaner, more viable and stable method than what is currently available. Currently, the few coal plants with commercial CO_2 capture capability all use processes based on chemical absorption with monoethanolamine (MEA), which unfortunately is nonselective, corrosive, requires the use of large equipment, and effective only under low to moderate partial pressures of CO_2. But the new system overcomes many of these shortcomings. Using ionic liquids as a separation solvent, however, has unique advantages over such solvents, according to Chemical Sciences Division scientist Amitesh Maiti, whose research appeared as the cover article in the July 2009 issue of ***ChemSusChem***, a new journal focused on chemistry and sustainability. Advantages include high chemical stability; low corrosion; almost zero vapor pressure; supportable on membranes; and a huge library of ion choices, which can be potentially optimized for CO_2 solubility. Maiti's work involved devising a computational strategy that can reliably screen any solvent, including an ionic liquid, for high CO_2 capture efficiency. "It's a great advantage to have a method that can quickly and accurately compute CO_2 solubility in any solvent, especially under the range of pressures and temperatures as would be found in a coal-fired power plant," Maiti said. "With ionic liquids serving as the solvent, the process could be a lot cleaner and more accessible than what is used today." Over the last few years several ionic liquids have been experimentally tested to be efficient solvents for CO_2, providing data that could be useful in optimizing the choice of ionic liquids for CO_2 capture. "But each new experiment costs time and money and is often hindered because a specific ionic liquid may not be readily available," Maiti said. "By creating a computational tool that can decipher ahead of time which ionic liquids work best to separate CO_2, it can be a much more efficient process when field tests are conducted." Maiti developed a quantum-chemistry-based thermodynamic approach to compute the chemical potential of a solute (CO_2 in this case) in any solvent at an arbitrary dilution. He found that this result coupled with an experimentally fitted equation-of-state data for CO_2 can yield accurate solubility values in a large number of solvents, including ionic liquids. He confirmed this by directly comparing the computed solubility with experimental values that have been gradually accumulating over the last few years. Next, he used this method to predict new solvent classes that would possess CO_2 solubility nearly two times as high as the most efficient solvents experimentally demonstrated. "With the vast choices of ions, we have barely scratched the surface of possibilities," Maiti added. His hope is that the accuracy of the computational method will allow scientists to see useful trends, which could potentially lead to the discovery of practical solvents with significantly higher CO_2 capture efficiency.

Contact: Amitesh Maiti (925) 422-6657 (maiti2@llnl.gov)

Shifting sound to light may lead to better computer chips

By reversing a process that converts electrical signals into sounds heard out of a cell phone, researchers may have a new tool to enhance the way computer chips, LEDs, and transistors are built. LLNL scientists have for the first time converted the highest frequency sounds into light by reversing a process that converts electrical signals to sound. Commonly used piezo-electric speakers, such as those found in a cell phone, operate at low frequencies that human ears can hear. But by reversing that process, lead researchers Michael Armstrong, Evan Reed and Mike Howard, LLNL colleagues, and collaborators from Los Alamos National Laboratory and Nitronex Corp., used a very high frequency sound wave—about 100 million times higher frequency than what humans can hear—to generate light. "This process allows us to very accurately 'see' the highest frequency sound waves by translating them into light," Armstrong said. The research appeared in the March 15 edition of ***Nature Physics*** and was also highlighted in the Fall 2009 issue of NNSA's ***Defense Science Quarterly***.

During the last decade, pioneering experiments using sub-picosecond lasers have demonstrated the generation and detection of acoustic and shock waves in materials with terahertz (THz) frequencies. These very same experiments led to a new technique for probing the structure of semiconductor devices. However, the recent research takes those initial experiments a step further by reversing the process, converting high-frequency sound waves into electricity. The researchers predicted that high-frequency acoustic waves can be detected by seeing radiation emitted when the acoustic wave passes an interface between piezoelectric materials. Very high-frequency sound waves have wavelengths approaching the atomic-length scale. Detection of these waves is challenging, but they are useful for probing materials on very small length scales. But that's not the only application, according to Reed. "This technique provides a new pathway to generation of THz radiation for security, medical and other purposes," he said. "In this application, we would utilize acoustic-based technologies to generate THz." Security applications include explosives detection and medical use may include detection of skin cancer. And the Livermore method doesn't

require any external source to detect the acoustic waves. "Usually scientists use an external laser beam that bounces off the acoustic wave—much like radar speed detectors—to observe high frequency sound. An advantage of our technique is that it doesn't require an external laser beam—the acoustic wave itself emits light that we detect," Armstrong said.

Contact: Michael Armstrong (925) 423-5702 (armstrong30@llnl.gov)

A green method to recycle a valuable explosive

Because of its many valuable properties, the high explosive 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) is used in about one-third of the nation's nuclear weapons, in some Department of Defense (DoD) munitions, and in explosives used by mining and oil production companies. However, TATB has not been produced for more than two decades primarily because of environmental regulations. As a result, DoD has been purchasing old TATB from Department of Energy (DOE) stockpiles while new, greener manufacturing methods are being developed. Until recently, a TATB recycling process was not available because effective solvents did not exist.

In response to urgent needs for replenished supplies of high-quality TATB, Livermore scientists have developed 3-ethyl-1-methylimidazolium acetate–dimethyl sulfoxide, a solvent system that belongs to a class of powerful but environmentally benign compounds called ionic liquids. This system has produced TATB with better crystal quality, size, shape, and purity than previous manufacturing techniques have produced. The new system may also have applications for efficiently converting cellulose and other difficult-to-dissolve organic compounds, such as cornstalks, into biofuels.

The TATB development effort was supported under the Transformational Materials Initiative (TMI), which focused on advanced materials for the nation's future nuclear stockpile. Its charter includes addressing critical issues such as the dwindling supply of high-quality TATB. The TMI-sponsored research on TATB was featured on the covers of the January 2009 issue of ***New Journal of Chemistry***. "TATB is a precious resource," says TMI leader Robert Maxwell, of the Chemical Science Division (CSD). "If we could recycle it when we disassemble warheads, we could save the nation many millions of dollars. However, we need exactly the right purity, particle size, and shape of TATB crystals to ensure the highest safety and performance standards."

Contact: Robert Maxwell (925) 423-4991 (maxwell7@llnl.gov)

New imaging technique reveals microbe metabolisms

The ability of microbes to absorb a wide range of substances has led DOE to investigate using microbes to develop biofuels, clean up toxics, and sequester carbon. However, to exploit microbial traits, scientists must better understand their growth and metabolism. "We want to determine how microbes react under different environmental conditions and how they could be engineered to perform useful functions," says Jennifer Pett-Ridge, an environmental microbiologist in CSD. Jennifer and her colleagues Peter Weber, Xavier Mayali, and Steve Singer worked with their collaborators at Stanford University to develop an imaging technique that identifies the microbes responsible for specific metabolic processes—elemental fluorescent in situ hybridization (El-FISH). The technique, which combines stable isotope probing with nanometer-scale secondary-ion mass spectrometry (NanoSIMS), shows which microbes in a given population use chemicals labeled with isotopes. The new technique thus allows researchers to study microbes in diverse environments, revealing the often-complex interrelationships of different species comprising microbial communities.

The isotope probing technique used is a variant of FISH, a technique that involves attaching fluorescent dyes to short pieces of DNA, called probes, which bind to complementary sequences of chromosomes in a targeted species. The technique can reveal the identities and locations of different microbes existing in complex communities. The twist of El-FISH is that an elemental tag, such as fluorine, attached to the probe is imaged in NanoSIMS along with the stable isotopes. First, the stable isotope—usually carbon-13 or nitrogen-15—provides information about how stable isotopes are metabolized, while the fluorine or bromine signal identifies the organism performing the metabolism.

In a DOE-funded collaboration with researchers at the National Aeronautics and Space Administration's Ames Research Center and Stanford University, Jennifer and her colleagues add compounds containing carbon-13 to microbial mat communities. They then follow how the bacteria take up and break down these compounds to learn about the critical links between carbon and nitrogen nutrients and the generation of hydrogen gas. The team is also partnering with Lawrence Berkeley National Laboratory and Louisiana State University to characterize the complex microbial community dwelling in the hindgut of wood-eating beetles. These beetles have developed a symbiotic relationship with a community of gut microbes whose combined enzymes digest the complex polysaccharides and lignins of plant cell walls and produce acetate, methane, and hydrogen gas. Understanding how these microbial populations interact to break down cellulosic materials could aid large-scale industrial projects planned to convert biomass such as wood chips into hydrogen and methane biofuels.

In a proof-of-concept demonstration of the El-FISH technique, the team imaged the assimilation and flow of nutrients between the two species of bacteria in a two-species community. A succession of NanoSIMS images reveals that carbon-13 is incorporated into cells through photosynthesis and nitrogen-15 through nitrogen fixation. (Four such images were chosen for the cover of the entire 2009 volume of the ***ISME Journal***.) El-FISH is now attracting interest from biological researchers worldwide. Over the next few years, scientists may use the technique to engineer bacteria for producing biofuels or to study microbial communities and host–pathogen interactions in nature and the human body. The methodology could also advance understanding of how microbes break down and sequester carbon dioxide in the soil, immobilize toxic metals, and biodegrade hazardous organic pollutants.

Contact: Jennifer Pett-Ridge (925) 424-2882 (pettridge2@llnl.gov)

Scientist publishes paper on N-doping of graphene in *Science*

As part of a collaboration led by Professor Hongjie Dai of Stanford University, chemist Peter Weber and colleagues have published a paper—"N-doping of graphene through electrothermal reactions with ammonia"—in the May 8, 2009 issue of ***Science***. Graphene has recently been made into semiconductors in the form of nanoribbons, leading to room-temperature P-type graphene field-effect transistors. However, a fundamental problem has been that the edge structures and chemical terminations of graphene synthesized by various methods are unknown and uncontrolled, whereas their effects on the physical properties have been widely predicted. In this paper, the team reports fabrication of a P-type graphene field-effect transistor that operates at room temperature. This research stems from a collaboration at Stanford University.

Contact: Peter Weber (925) 422-3018 (weber21@llnl.gov)

Securing radiological sources

Keeping radiological materials out of the hands of potential terrorists and other adversaries is the goal of the National Nuclear Security Administration's Global Threat Reduction Initiative (GTRI), which is tasked with reducing and protecting vulnerable nuclear and radiological materials at civilian sites worldwide. GTRI works closely in this endeavor with the International Atomic Energy Agency (IAEA), which issues international standards and guidance on how to safely control radioactive sources. Lawrence Livermore researchers have been active contributors to GTRI for years.

CSD health physicist Carolyn Mac Kenzie, who leads the Livermore team, spent three years at the IAEA in Vienna, Austria, and another year on assignment at NNSA's GTRI headquarters in Washington, DC, as a Livermore contractor. She returned to the Laboratory in October 2007. While in Vienna, she led the IAEA Orphan Source Search and Secure Program and worked in more than 35 countries to establish strategic plans for locating and securing

(left) Livermore's Tim Horgan visits a source storage facility. (right, top) A local contractor tests security upgrades installed at a hospital. (right, bottom) Livermore's Carolyn Mac Kenzie and Zephrin Ouedraogo, a radiation protection regulatory authority in Burkina Faso, examine a tsetse-fly irradiator.

orphan and legacy radiological sources. When Mac Kenzie left the IAEA to work at GTRI in Washington, DC, she continued her efforts to locate and secure sources in Africa. Since returning to the Laboratory, her team has worked through GTRI in seven countries: Burkina Faso, Gabon, Ghana, Democratic Republic of Congo, Mauritius, Namibia, and the Republic of Congo. “We had started a project in Madagascar but a coup derailed our work,” says Mac Kenzie. “We are awaiting more peaceful times before returning.”

Contact: Carolyn Mac Kenzie (925) 422-7618 (mackenzie5@llnl.gov)

Researchers help investigate deep mantle under Tibet

A paper by Larissa Dobrzhinetskaya (UC Riverside) and others including PLS geochemists Ian Hutcheon and Peter Weber (both of CSD) appeared in the October 30 online edition of the ***Proceedings of the National Academy of Sciences***. The paper, titled “High-pressure, highly reduced nitrides and oxides from chromitite of a Tibetan ophiolite,” reports on fragments of a highly reduced deep mantle environment from a depth of at least 300 km and has implications for the oxygen fugacity in the deep earth. Isotopic compositions of nitrogen and carbon were measured using LLNL’s NanoSIMS. The findings were strengthened by observation of coesite and diopside lamellae within chromite collected from the same outcrop. In addition, diamonds and other mineral indicators of very low oxygen fugacity were found in a second ophiolite in the Polar Ural Mountains that would imply that the Tibetan occurrence is not unique.

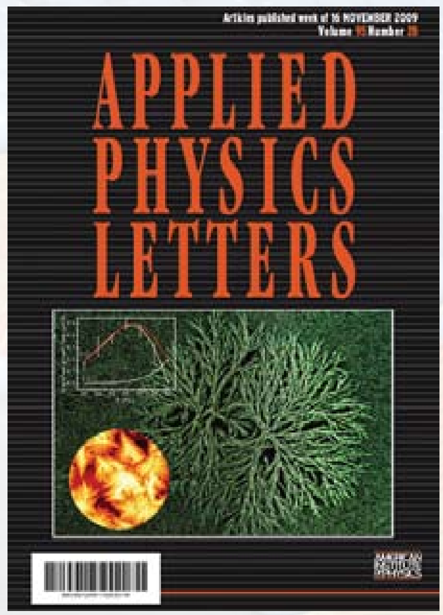
Contacts: Ian Hutcheon (925) 422-4481 (hutcheon1@llnl.gov) and Peter Weber (925) 422-3018 (weber21@llnl.gov)

Aerosol mass spectrometry technique for drug identification

A paper published in the October 20, 2009 edition of ***Analytical Chemistry*** expands the application of single-partical aerosol mass spectrometry (SPAMS) to detect and identify multicomponent drug tablets and mixed drug tablet samples. The title of the paper is “Use of single-particle aerosol mass spectrometry for the automated nondestructive identification of drugs in multicomponent samples.” The original development of the SPAMS system at LLNL was partially funded through Laboratory Directed Research and Development Program funds. LLNL co-authors include Audrey Martin (CSD), George Farquar (BBTD), Paul Steele (Physics), and Matthias Frank (Physics).

Contact: Audrey Martin (925) 423-4675 (martin210@llnl.gov)

Research featured on *APL* cover



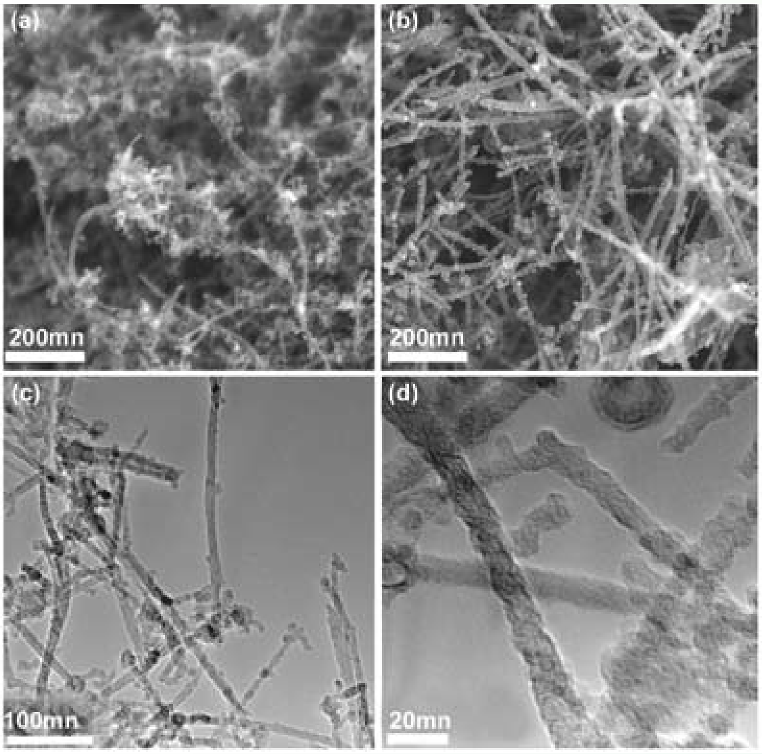
Richard Gee and Amitesh Maiti, both of PLS, are coauthors of a paper—“Fractal growth in organic thin films: Experiments and modeling”—featured on the cover of the November 16, 2009 issue of ***Applied Physics Letters***. The cover (above) shows an optical microscope image of an energetic material that spontaneously arranges into a dendritic pattern. The round inset is a close-up of the self-similar, fractal-like features of one of the dendrite branches, with fractal dimensions characteristic of diffusion-limited aggregation. The graph shows the growth rate of one of the branches as a function of temperature. The paper described the investigation of fractal growth of pentaerythritol tetranitrate (PETN) films that were thermally deposited on a silicon substrate.

Gee, Maiti, and their two colleagues (Gengxin Zhang and Brandon Weeks) from the Texas Tech University developed a simple theoretical model to show how such patterns can be explained on the basis of competing effects of diffusion-mediated aggregation and desorption of molecules. Findings reported in the paper should help in the understanding of growth kinetics and coarsening processes in PETN and other organic materials.

Contacts: Richard Gee (925) 423-1177 (gee10@llnl.gov) and Amitesh Maiti (925) 422-6657 (maiti2@llnl.gov)

Carbon nanotube foams that simultaneously exhibit high electrical conductivities and robust mechanical properties fabricated

In a paper published in ***Applied Physics Letters*** (Vol 94, 2009), the fabrication of low-density carbon nanotube (CNT) foams that simultaneously exhibit remarkable mechanical stiffness, very large elastic strains, and high electrical conductivity is described. One of the critical aspects in the design was the selection of the binder or "glue" used to reinforce the low-density CNT structures. The new approach was to use carbon nanoparticles to crosslink randomly oriented bundles of single-walled CNTs, affording ultralow-density nanoporous monoliths as low as 10 mg cm^{-3} with unprecedented properties. The foams are the stiffest low-density nanoporous solids reported and exhibit elastic behavior up to compressive strains as large as 80%. The use of carbonaceous binder also allows bulk electrical conductivity to be maintained at low densities. In addition, this process provided the versatility to generate monolithic CNT foams in conformable shapes for different applications. The CNT foams were prepared using highly purified single-walled CNTs, as these nanotubes are readily suspended in water using sonication without surfactants or other additives that are typically required to disperse CNTs in aqueous media. To reinforce the CNT network, organic sol-gel chemistry was used to form carbonaceous interconnections between the CNTs. Organic sol-gel chemistry can be used to prepare a variety of mesoporous materials, including carbon aerogels. The process typically involves the polymerization of organic precursors to produce highly crosslinked organic gels that can then be dried and pyrolyzed to yield porous carbon structures. In this case, however, the process is used to make the conductive glue that holds the CNT assembly together. By introducing low concentrations of the sol-gel precursors to a suspension of highly purified single-walled CNTs, polymerization was induced primarily on the walls of the CNT bundles and, more importantly, at the junctions between adjacent bundles to form an organic binder. The resulting assembly can then be dried and subsequently pyrolyzed to convert the organic binder to carbon.



Scanning electron microscopy images of carbon nanotube (CNT) foams containing (a) 30wt % and (b) 55wt % CNTs and transmission electron micrscopy images [(c) and (d)] at different magnifications of a foam containing 30wt % CNT.

Contact: Marcus Worsley (925) 424-4831 (worsley1@llnl.gov)

Enhanced thermal transport in carbon aerogel with nanotubes measured

In a paper published in the online April 29, 2009 edition of ***Journal of Applied Physics***, chemists

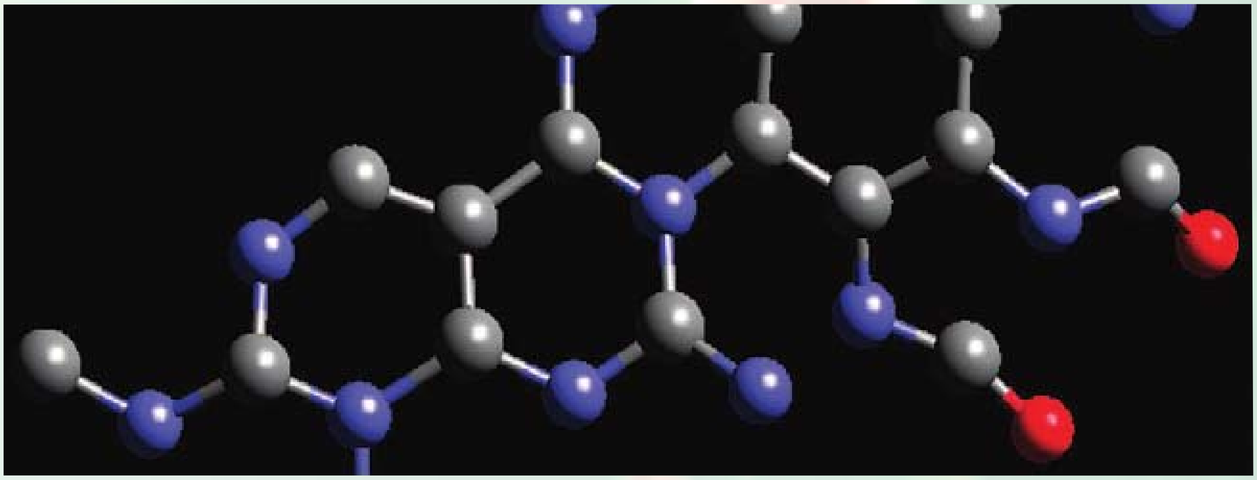
Marcus Worsley, Joe Satcher, and Theodore Baumann describe thermal conductivity measurements of a carbon aerogel nanocomposite containing double-walled carbon nanotubes. The nanocomposites were prepared by the sol-gel polymerization of resorcinol with formaldehyde in aqueous suspension containing a surfactant-stabilized dispersion of double-walled carbon nanotubes. Subsequent drying and pyrolysis resulted in free-standing monolithic carbon aerogel nanocomposites with uniform dispersions of carbon nanotubes. The monoliths were characterized by high-resolution scanning electron microscopy and thermal conductivity measurements via the transient hot-wire method. Enhanced thermal conductivities were observed for carbon aerogel nanocomposites relative to pristine carbon aerogels.

Contacts: Marcus Worsley (925) 424-4831 (worsley1@llnl.gov), Joe Satcher (925) 422-7794 (satcher1@llnl.gov), and Theodore Baumann (925) 423-5543 (baumann2@llnl.gov)

The first quantum-based multiscale simulations to study reactivity of shocked perfect crystals of triaminotrinitrobenzene (TATB)

As reported in the March edition of the ***Journal of the American Chemical Society***, the reactivity of crystal material triaminotrinitrobenzene (TATB) was simulated under steady overdriven shock compression using the multiscale shock technique. In this molecular dynamics method, equations of motion for the atoms and volume of the computational cell are time evolved subject to stress and energy constraints satisfying a continuum description of the shock wave. Since the computational cell of the multiscale technique follows a Lagrangian point through the shock wave, it enables a simulation of a system experiencing a shock wave with far fewer atoms than normally required by the direct method of inducing a shock wave in a very large computational cell. In tandem, the use of quantum based methods to calculate interatomic forces allows reliable predictions of chemical reactions, while providing insights into the electronic structure and chemical transformations of the reacting system for a relatively long time scale—on the order of several hundreds of picoseconds. As reported in the paper, tracking chemical transformations of TATB experiencing overdriven shock speeds of 9 km/s for up to 0.43 ns and 10 km/s for up to 0.2 ns reveal high concentrations of nitrogen-rich heterocyclic clusters. Further reactivity of TATB toward the final decomposition products of fluid N_2 and solid carbon is inhibited due to the formation of these heterocycles. Results suggest a new mechanism for carbon-rich explosive materials that precedes the slow diffusion-limited process of forming the bulk solid from carbon clusters and provide fundamental insight at the atomistic level into the long reaction zone of shocked TATB.

Contact: Riad Manaa (925) 423-8668 (manaa1@llnl.gov)



Representative nitrogen-rich heterocycle near the end of simulated TATB experiencing a steady shock wave with a speed of 9 km/s.

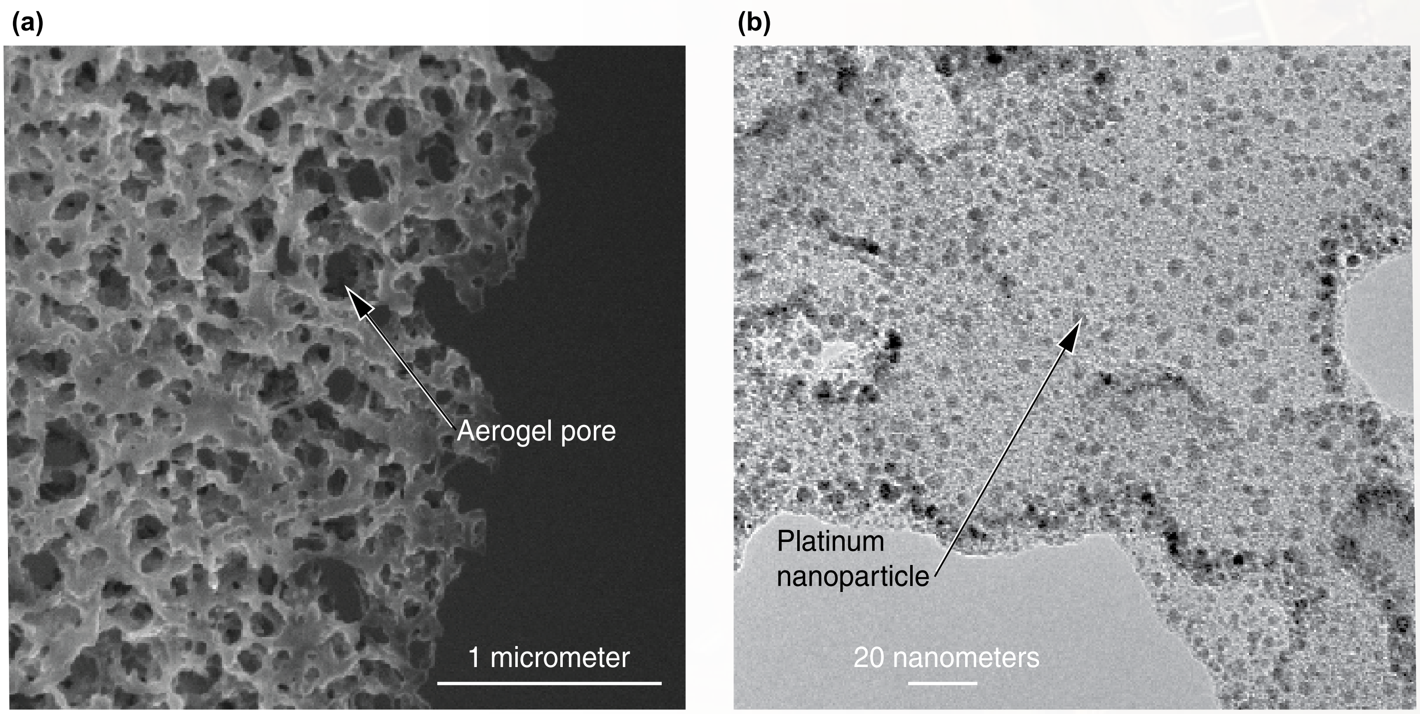
Materials Sciences

Doped aerogels demonstrate performance and show promise

Aerogels—highly porous, extremely low-density, structures—have become exceedingly useful at the Laboratory in laser target fabrication, energetic composites, sensors, ceramics, and coatings. Doping is used to impart additional chemical elements into the matrix. However, this doping process can be challenging because of aerogel's complex pore structure. Recently, a team of Livermore researchers helped develop an efficient method to dope carbon aerogel with platinum, which is an effective catalyst with many possible applications. Platinum's cost, however, limit such applications. However, using atomic layer deposition (ALD)—a gas deposition process that provides atomic-level control of thin films—a Livermore team added minute amounts of platinum to uniform discs of carbon aerogel.

Incorporating catalyst particles into aerogels in a controlled fashion can be challenging because of the material's extremely small pore networks. According to Juergen Biener, a materials scientist in PLS's Nanoscale Synthesis and Characterization Laboratory who led the project, "Nanoporous materials can be difficult to dope without interfering with their structure. However, the self-limiting character of the ALD process is ideally suited for depositing particles in nanoporous materials with atomic-level control."

The platinum ALD experiments were conducted at Stanford University. CMMD team members Sergei Kucheyev and Morris Wang characterized the 10-cycle platinum-loaded aerogels at Livermore using Rutherford backscattering spectrometry and cross-sectional transmission electron microscopy. The characterization revealed that the deposited



(a) A cross-sectional micrograph from a scanning electron microscope shows the high porosity of carbon aerogels. This sample was treated with platinum using 10 atomic layer deposition cycles. (b) A higher magnification micrograph from a transmission electron microscope reveals the deposition of platinum nanoparticles with an average size of 2.4 nanometers.

platinum does not form a continuous thin film on the surface of the carbon aerogel. Rather, the platinum–aerogel interaction produces hemispherical platinum nanoparticles less than 5 nanometers in diameter. Forming such small platinum nanoparticles is key to a high catalytic efficiency because more of the catalyst's atoms are exposed at the surface, thus increasing the catalyst's ability to induce chemical reactions.

The catalytic properties of the platinum-loaded aerogels were then tested at the University of Bremen. The team compared the conversion rates of each of the aerogels for oxidizing the carbon monoxide into carbon dioxide. Surprisingly, they found the aerogel that had undergone only two ALD cycles—which deposited as little as 0.05 milligrams of platinum per square centimeter—had the same conversion efficiency—nearly 100 percent conversion in the 150 to 250°C range—as those that had been through 5 and 10 cycles. In other words, less platinum could be used to obtain the same catalytic effect.

Team member Ted Baumann, whose interest in the work was directly related to his work on a DOE–funded project for hydrogen storage, led the platinum catalysis experiments. Baumann and Biener have also explored the potential of other nanoporous materials such as gold for use in catalytic and other applications. According to these scientists, the potential use for nanoporous materials is virtually untapped. As Baumann, Biener, and other researchers continue their work on nanoporous structures, the scientific and technological innovations they bring about could have a significant effect on the way electric, catalytic, and waste management processes are performed today. In the future, nanoporous materials such as platinum-loaded aerogels could play a key role in applications for water treatment, hydrogen storage technology, and more efficient fuel cells that use less but do more.

Contacts: Juergen Biener (925) 422-9081 (biener2@llnl.gov) and Ted Baumann (925) 423-5543 (baumann2@llnl.gov)

Hydrogen–helium mixtures in Saturn and Jupiter interiors elucidated

By determining the properties of hydrogen–helium under conditions found in the interiors of Saturn and Jupiter, LLNL physicists, in collaboration with the University of Illinois at Urbana-Champaign, have determined the temperature at a given pressure at which helium becomes insoluble in dense metallic hydrogen. The results were published in the February 3, 2009 edition of the ***Proceedings of the National Academy of Sciences***. Using first-principles molecular dynamics simulations, Miguel Morales and David Ceperley at the University of Illinois; LLNL's Eric Schwegler, Sebastien Hamel, and Kyle Caspersen (of PLS); and Carlo Pierleoni of the University of L'Aquila in Italy determined the equation of state of the hydrogen–helium system at extremely high temperatures (4,000–10,000 degrees Kelvin), similar to what would be found in the interior of Saturn and Jupiter. The team used LLNL's high-performance computing facilities to conduct simulations over a wide range of density, temperature, and composition to locate the equation of state of the two elements.

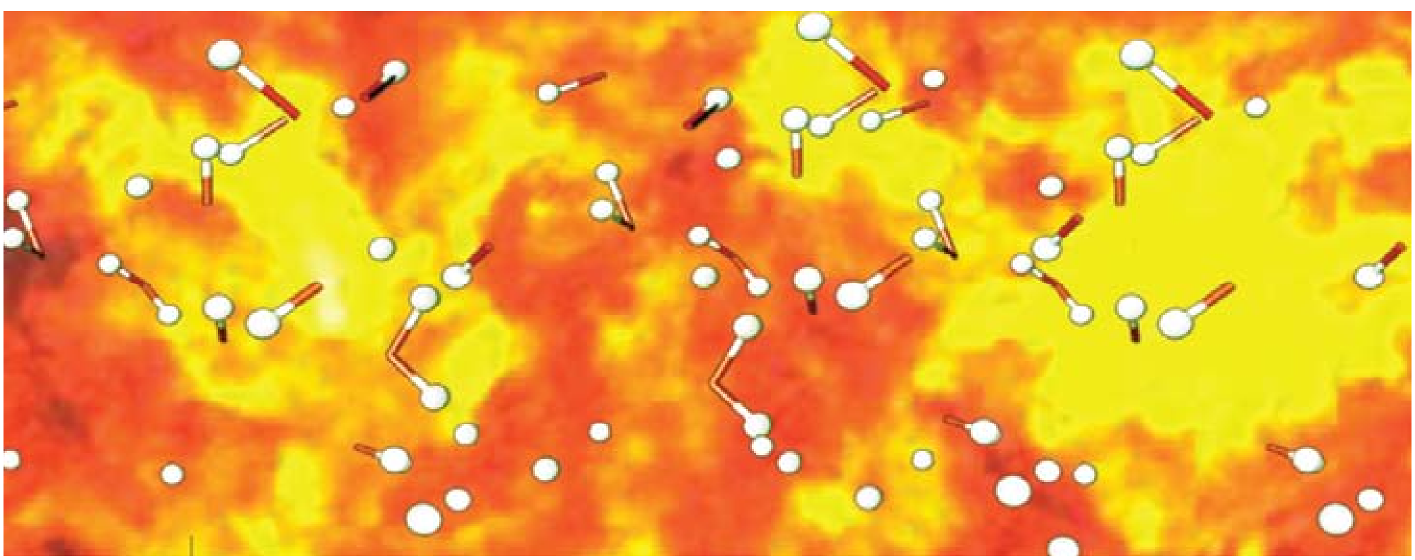
Contact: Eric Schwegler (925) 424-3098 (schwegler1@llnl.gov)

Water acts as catalyst in explosives

The most abundant material on Earth exhibits some unusual chemical properties when placed under extreme conditions. LLNL scientists have shown that water, in hot dense environments, plays an unexpected role in catalyzing complex explosive reactions. A catalyst is a compound that speeds chemical reactions without being consumed. Platinum and enzymes are common catalysts. But water rarely, if ever, acts as a catalyst under ordinary conditions.

Detonations of high explosives made up of oxygen and hydrogen produce water at thousands of degrees Kelvin and up to 100,000 atmospheres of pressure, similar to conditions in the interiors of giant planets. While the properties of pure water at high pressures and temperatures have been studied for years, this extreme water in a reactive environment has never been studied. Until now. Using first-principle atomistic simulations of the detonation of the high explosive PETN (pentaerythritol tetranitrate), the team discovered that in water, when one hydrogen atom serves as a reducer and the hydroxide (OH) serves as an oxidizer, the atoms act as a dynamic team that transports oxygen between reaction centers. “This was news to us,” said lead researcher Christine Wu. “This suggests that water also may catalyze reactions in other explosives and in planetary interiors.” This finding is contrary to the current view that water is simply a stable detonation product. “Under extreme conditions, water is chemically peculiar because of its frequent dissociations,” Wu said. “As you compress it to the conditions you’d find in the interior of a planet, the hydrogen of a water molecule starts to move around very fast.”

In the molecular dynamic simulations using the Lab’s BlueGene/L supercomputer, Wu and colleagues Larry Fried, Lin Yang, Nir Goldman, and Sorin Bastea found that the hydrogen atoms and OH molecules in water transport oxygen from nitrogen storage to carbon fuel under PETN detonation conditions (temperatures between 3,000 Kelvin and 4,200 Kelvin). Under both temperature conditions, this “extreme water” served both as an end product and as a key chemical catalyst. For a molecular high explosive that is made up of carbon, nitrogen, oxygen and hydrogen, such as PETN, the three major gaseous products are water, carbon dioxide and molecular nitrogen. But to date, the chemical processes leading to these stable compounds are not well understood. The team found that nitrogen loses its oxygen mostly to hydrogen, not to carbon, even after the concentration of water reaches equilibrium. They also found that carbon atoms capture oxygen mostly from hydroxide, rather than directly from nitrogen monoxide or nitrogen dioxide. Meanwhile water



Simulation of water acting as a catalyst in an explosion.

disassociates and recombines with hydrogen and hydroxide frequently. "The water that comes out is part of the energy release mechanism," Wu said. "This catalytic mechanism is completely different from previously proposed decomposition mechanisms for PETN or similar explosives, in which water is just an end product. This new discovery could have implications for scientists studying the interiors of Uranus and Neptune where water is in an extreme form." The research appeared in the premier issue (April 2009) of ***Nature Chemistry***.

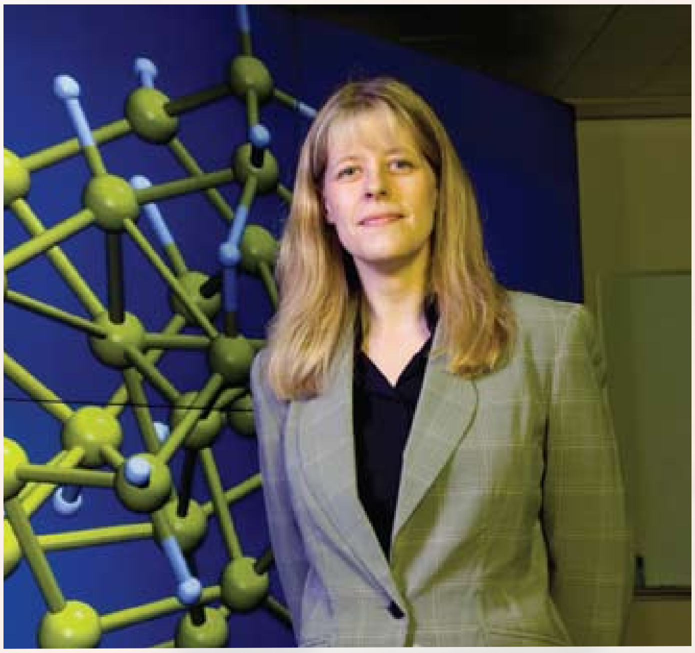
Contact: Christine Wu (925) 424-4096 (wu5@llnl.gov)

Understanding the surface structure of nanomaterials

Computer simulations play a significant role in helping researchers understand the functions of materials and living organisms. Postdoctoral researcher Heather Whitley has worked with fellow CMMD scientists Eric Schwegler and Tadashi Ogitsu using Livermore's advanced computing resources to study the properties of nanomaterials under pressure, the effects of surface structure on the x-ray absorption spectra of a nanomaterial, and materials designed for quantum computers.

When a material shrinks to nanometer size (10^{-9} meters), its surface has an increased influence on its physical and optical properties as well as its crystalline structure. Using quantum mechanical simulations, Whitley examined the size dependence of pressure-induced structural phase transitions in silicon quantum dots. "Understanding fundamental properties at a microscopic level is key to developing new technologies based on semiconductor nanomaterials," says Whitley. In addition, she is collaborating with researchers from Lawrence Berkeley National Laboratory to calculate the x-ray absorption spectra of cadmium–selenium nanomaterials.

Whitley is also working with UC Berkeley on a detailed computational analysis of materials for quantum computing. "A major barrier to developing quantum computers is decoherence, a process by which information encoded in a quantum state is lost because of interactions between the quantum system and its surroundings," says Whitley. The group's findings from previous experimentation using phosphorus-31 suggest that the donor electron spin state, which has a fast response to an external field, could be used to perform fast quantum operations. Information encoded in the electron spin state could be transferred to the nuclear spin state, which has a longer lifetime, to enable efficient readout of quantum information. Collaborators at Lawrence Berkeley are also investigating the proposed design to determine which materials are suitable for building a quantum computer.



Heather Whitley uses the Laboratory's advanced computing resources to study nanomaterials.

Working with professionals in her field has opened Whitley's eyes to its many possibilities. "I've seen what science is like outside academia," she says. "Plus, I've had an opportunity to use some of the most advanced computational equipment in existence. I don't think I could have ended up in a better place."

Contact: Heather Whitley (925) 422-1741 (whitley3@llnl.gov)

Postdoc investigates crystal growth for diverse Lab missions

With a Ph.D. in chemical engineering, postdoctoral researcher Selim Elhadj has contributed to a diverse array of programs, from NIF to biosciences. "I was brought to the Laboratory because of my knowledge of crystal growth processes, which are essential for understanding the structural dynamics of nonlinear optical materials and, surprisingly, biological membranes," says Elhadj.

Using atomic force microscopy (AFM), he helped develop a method for mitigating damage on laser optics. With colleagues Vaughn Draggoo, Alex Chernov, and then-LLNL employee Jim De Yoreo, Elhadj placed a laser-damaged potassium–dihydrogen–phosphate (KDP) crystal substrate into a tightly controlled atmosphere. As the meniscus passed over imperfections in the crystal, KDP molecules were dissolved from convex features and precipitated in concave ones. This redistribution of material was thermodynamically driven and well predicted by a form of the Gibbs–Thomson law, which relates surface curvature to vapor pressure and chemical potential. Says Elhadj, "The mitigation method relies on the shape-dependent solubility of the features, the contrast in their local solubility, and the molecular fluxes within the solvent layer."

Elhadj has also worked with Ibo Matthews and Steven Yang to research methods that will mitigate defects in silica optics by using lasers to melt and vaporize silica.

Selim Elhadj's expertise in crystal growth processes supports a diverse range of Laboratory programs.

"We used thermographic techniques to measure the temperature of the laser-exposed surfaces," he says. "We then included these measurements in models to predict how the optical materials change and to build diagnostic tools for process control. Measuring the temperature is essential because it represents the driving force of the observed changes relevant to laser-based mitigation."

Contacts: Selim Elhadj (925) 422-0270 (elhadj2@llnl.gov)

Actinide research published in *Reviews of Modern Physics*

A Livermore researcher who teamed with a United Kingdom collaborator has published an article in ***Reviews of Modern Physics*** that refines decades of actinide science and may just become the pre-eminent research paper in the field. Kevin Moore of LLNL and Gerrit van der Laan at the Diamond Light Source in the United Kingdom wrote "Nature of the 5f states in actinide metals," which describes the electronic, magnetic and crystal structure of actinides and demonstrates the importance of actinide science to a broad class of scientists. It appeared in the journal's February 6, 2009 edition.

Actinides encompass the 15 chemical elements that lie between actinium and lawrencium included on the periodic table, with atomic numbers 89–103. The actinide series derives its name from the first element in the series, actinium. The 5f states are complicated electron wave functions. ***Reviews of Modern Physics*** is the premier journal for physics research. It is the fifth highest ranked journal out of all fields and only publishes 32 invited papers a year. Each year, one or more of the invited papers are used in part as acceptance speeches for the Nobel Prize in physics. Moore and van der Laan's paper points out that the heaviest actinides have almost no experimental data, generating only a rudimentary level of understanding. "The actinide series as a whole is modestly understood, with the level of comprehension decreasing with atomic number," Moore said. While theoretical work on the actinides is substantial, the lack of experiments is due to the toxic and radioactive nature of the materials, which makes handling difficult and expensive. In addition, the cost of the materials themselves is exceedingly high, meaning experiments that need a large amount of materials further increase the expense of research. Progress in understanding the theoretical calculations has its limits as well. It's been hampered by the extreme difficulty of the physics and the lack of a healthy body of experimental data from which to validate the theory. However, Moore and van der Laan explain the progress in understanding the electronic structure of the 5f states in the actinide metal series by sifting through decades of research in the theoretical and experimental fields and condensing the data in a definitive article on actinide science. "This establishes LLNL as a frontrunner in actinide science and highlights the work done at defense labs by having that research in a world-class journal," Moore said.

Contact: Kevin Moore (925) 422-9741 (moore78@llnl.gov)

Nanocrystal results published in ACS journals and *Nature*

Nanomaterials continue to exhibit new and unexpected physical properties that are both of fundamental scientific interest and considerable technological value. PLS scientists have recently reported important breakthroughs in understanding the behavior of cadmium selenide (CdSe) nanocrystals, a model system among nanocrystalline semiconductors, in two American Chemical Society (ACS) journals. In the first paper—published in the ***Journal of the American Chemical Society*** and featured in the Research Highlights section of the May 21, 2009 edition of ***Nature***—the research team report magnetic properties in nanocrystalline CdSe that are not observed in the bulk material and demonstrate that the magnetic susceptibility can be manipulated by varying the particle size and surface chemistry. This work, carried out in collaboration with Argonne National Laboratory and the

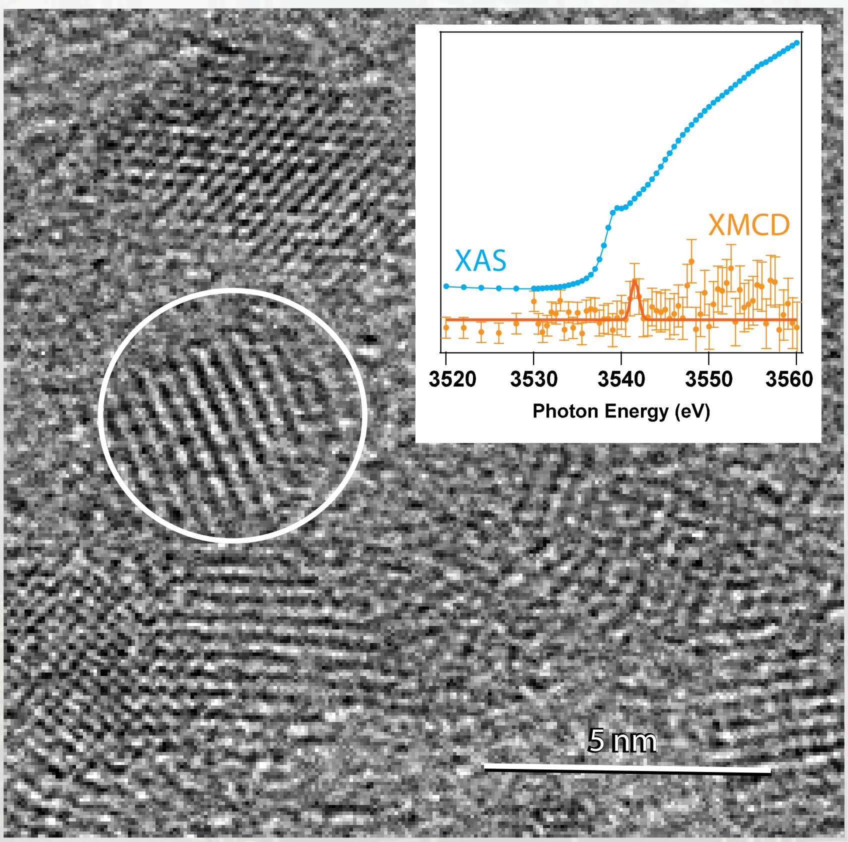
Naval Research Laboratory, resolves controversy in the literature regarding the origin of magnetism in nanoscale CdSe, which could have significant implications for the development of designer magnetic nanomaterials. The second paper, published in ***ACS Nano***, describes the first-ever experimental determination of the size-dependent exciton binding energy of CdSe nanocrystals, which provides a reference point for evaluating extensive theoretical modeling on the subject. The scaling of the exciton binding energy with size has been long sought after because of its importance in understanding the optical properties of nanocrystalline CdSe and was determined as part of a collaboration with researchers at UC Santa Cruz.

Contact: Jonathan Lee (925) 422-5846 (lee204@llnl.gov)

Paper published on hydrogen embrittlement in metals

A paper—"Grain-boundary engineering markedly reduces susceptibility to intergranular hydrogen embrittlement in metallic materials"—was published in ***Acta Materialia*** as a culmination of a long-standing collaboration between Mukul Kumar (CMMD) and Rob Ritchie of UC Berkeley and LBNL. This paper clearly demonstrates the utility of manipulating microstructural topologies (in metallic systems) to markedly enhance its resistance to hydrogen-induced intergranular embrittlement. This research has practical application for material design in a hydrogen-based energy system.

Contact: Mukul Kumar (925) 422-0600 (kumar3@llnl.gov)



A transmission electron microscopy image of cadmium selenide (CdSe) nanocrystals coated with trioctylphosphine oxide (TOPO) surfactants. The image clearly illustrates both the nanocrystals' size (3 nm in diameter) and crystallinity. The white circle surrounds a representative CdSe–TOPO nanocrystal. The inset table graphs data obtained with Cd L3-edge x-ray magnetic circular dichroism (orange) and x-ray absorption spectroscopy (blue). The former signal indicates that the magnetic susceptibility is associated with Cd atoms in the nanocrystals, while the latter data elucidate the unfilled electronic states in the CdSe–TOPO and were crucial in determining exciton binding energy.

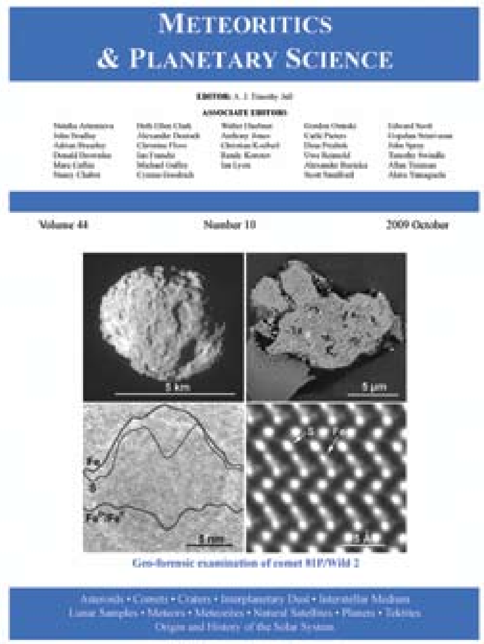
Scientist contributes to refrigeration materials research

Scott McCall, of CMMD, with colleagues at Tuskegee University (now at San Jose State), Sandia National Laboratory, and Rutgers University, published a paper—"Enhanced magnetic refrigeration capacity in phase separated manganites"—in the August 31, 2009 issue of ***Applied Physics Letters***. Magnetic refrigeration is a promising solid-state alternative for cooling, as it is potentially more efficient than gas phase compression–expansion processes and does not involve harmful emissions. Success will depend on developing materials with a large magnetocaloric effect to realize efficient magnetic refrigeration. This research has shown that magnetic phase separation in a single material can be used to widen the temperature range of the magnetocaloric effect, improving regenerative magnetic refrigerator designs.

Contact: Scott McCall (925) 422-1499 (mccall10@llnl.gov)

Stardust sample images featured

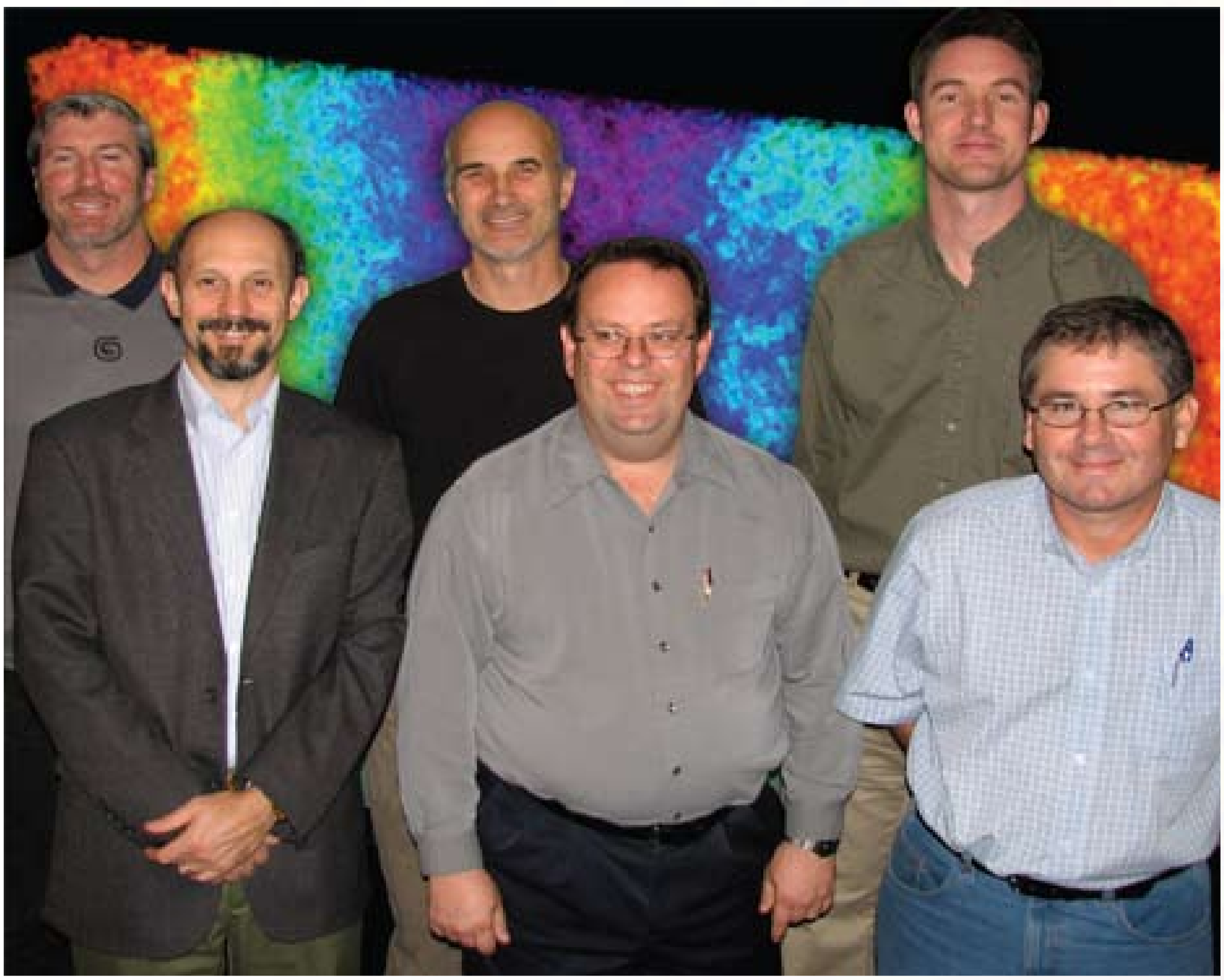
The October 2009 issue of ***Meteoritics and Planetary Science*** features on its cover images made at LLNL using super scanning transmission electron microscopy and scanning electron microscopy. MAPS is considered the flagship journal of the planetary materials and mission science communities. The October issue contains 17 papers from the 2008 Timber Cove conference sponsored by the Institute for Geophysics and Planetary Physics (IGPP). Three of the 17 papers were written by PLS authors—Penny Wozniakiewicz, Hope Ishii (both of CMMD), Zurong Dai (CSD), and John Bradley. In addition, Bradley wrote the guest editorial for the issue. The Timber Cove conference was so successful that NASA has agreed to fund another meeting, which is being organized by IGPP Director John Bradley and will be held in February 2011.



Contact: Penny Wozniakiewicz (925) 424-2581 (penny-w@llnl.gov)

"Impossible" calculation presented at conference

Taking on a charged particle physics calculation previously labeled "impossible," a team of Lab scientists led by CMMD physicist Jim Glosli developed an unorthodox strategy to exploit the power of massively parallel supercomputers and break new ground in scientific simulation. The multidisciplinary team, which included an IBM researcher, presented its methodology at ***Supercomputing 2009***, the premier high-performance computing conference, held in Portland, OR, Nov. 16–20. They were also finalists for the prestigious Gordon Bell Prize. The new BlueGene/P node technology allowed them to use this new approach—called heterogeneous decomposition—to more fully exploit the system's capabilities. This new capability was developed by scientists in Computation's Institute for Scientific Computing Research (ISCR) on two IBM BlueGene/P systems—the 500-teraflops Dawn at the Lab and the 1.03-petaflops Jugene at Germany's Julich Supercomputing Center. "Our institute's mission is to advance the state of the art for applications of national interest," said Fred Streitz (CMMD), ISCR director. "In this case we focused on scaling a simulation that involved the calculation of long-range forces. Some people said that this was impossible—but this very talented team proved the naysayers wrong." Jim Glosli, project leader, said this development has farreaching implications for scientific computing and will likely affect the way future codes are developed. "What is innovative



is the different way we broke up the machine to run the calculation. This allows more complicated models and this approach can be applied to other applications," Glosli said. "The flexible approach we've been able to demonstrate will allow many problems to scale across both current and next-generation machines." Shown in the photo are, left to right, Liam Krauss, Fred Streitz, Jim Glosli, David Richards, Erik Draeger, and Tom Spelce.

Contacts: Fred Streitz (925) 423-3236 (streitz1@llnl.gov) and Jim Glosli (925) 422-5849 (glosli1@llnl.gov)

Work upends conventional view of transition metals

CMMD physicists Alex Landa and Per Söderlind have, with colleagues from Sweden's Royal Institute of Technology, discovered features of the transition metals that contradict conventional explanations for their phase stability. Their findings were published in a paper—"Stability in bcc transition metals: Madelung and band-energy effects due to alloying"—in the December 4, 2009 issue of ***Physical Review Letters***.

Contacts: Alex Landa (925) 424-3523 (landa1@llnl.gov) and Per Söderlind (925) 423-4667 (soderlind1@llnl.gov)

Results on tantalum plastic flow published

A research paper by CMMD scientists Christine Wu, Per Söderlind, James Glosli, and John Klepeis—"Shear-induced anisotropic plastic flow from body-centered-cubic tantalum before melting"—was published in the March 2009 edition of ***Nature Materials***. As reported by Wu et al., "There are many structural and optical similarities between a liquid and a plastic flow. Thus, it is non-trivial to distinguish between them at high pressures and temperatures . . . . We report a shear-induced, partially disordered viscous plastic flow from body-centered-cubic tantalum under heating before it melts into a liquid . . . [that] offers a plausible resolution to a long-standing controversy about melting of metals under high pressures."

Contact: Christine Wu (925) 424-4096 (wu5@llnl.gov)

Earth Sciences

Geothermal energy program sees renewal in three projects

In early 2009, DOE's Office of Energy Efficiency and Renewable Energy issued a call for proposals from $400,000 to $600,000 per year for three years under Recovery Act funding for geothermal research. Each national lab was allowed to submit four proposals. LLNL had three out of four proposals of its geothermal project proposals selected for funding. One of the three projects focuses on developing realistic computer-based models of enhanced geothermal system (EGS) stimulation-response scenarios. EGS is the creation of an effective subsurface heat exchanger for power generation when the natural system is hot enough but fracture permeability is insufficient. The simulations are aimed at assessing the influence of many EGS properties, such as rock formation mechanical characteristics, initial thermal and stress state of the targeted rock formation, and hydraulic and explosive modes of fracture propagation, among others.

Steampipe to a geothermal plant in The Geysers, Sonoma County, CA. (Photo courtesy of Don Follows, Yellowstone National Park.)

The second project will map microseismicity for geothermal reservoir management. The project is aimed at detecting and locating microearthquakes induced by EGS hydrofracturing and fluid reinjection operations within the reservoirs. In EGS, water is initially pumped into the ground at high pressures. After the underground fracture network is developed, cold water can be reinjected at lower pressures, heated by the host rock, and extracted from a production well as extremely hot water. This hot water can then be converted into electricity in geothermal power plants. Using seismic tools, the team can locate where the cracks are initially forming and the possible locations of the reinjected fluids by tracking the microseismicity.

The third project determines what effect geochemical reactions have on the use of carbon dioxide (CO_2) as an efficient heat exchanger for geothermal energy production. Earlier research had shown that using supercritical CO_2 instead of water as a heat transfer fluid yields significantly greater heat extraction rates for geothermal energy. If successful, this technology could increase geothermal energy production and offset atmospheric emissions of greenhouse gases, although the impact of geochemical reactions between acidic waters in equilibrium with supercritical CO_2 and the reservoir rock has not been assessed.

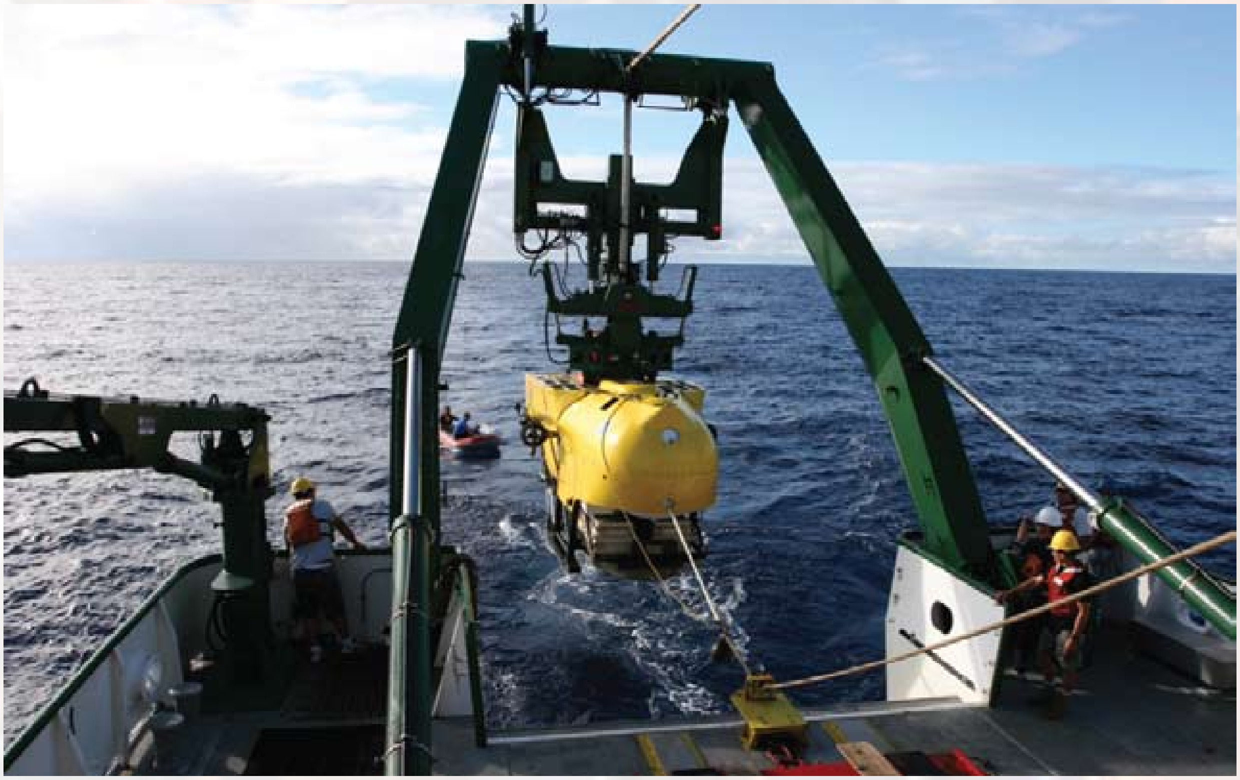
DOE's budget for geothermal energy has fluctuated during the last decade going from about $22 million per year, down to $5 million in 2007 and then bounced up to $44 million this year. As commented by Jeff Roberts, LLNL geothermal program leader, "People have realized that climate change is a real issue. Everything has changed to work in favor of getting more renewable energy moving forward."

Contact: Jeff Roberts (925) 422-7108 (roberts17@llnl.gov)

Deep sea corals shown to be possibly oldest living marine organism

Deep-sea corals from about 400 meters off the coast of the Hawaiian Islands are much older than once believed and some may be the oldest living marine organisms known to man. Researchers from LLNL, Stanford University, and the University of California at Santa Cruz have determined that two groups of Hawaiian deep-sea corals are far older than previously recorded. Using the Lab's Center for Accelerator Mass Spectrometry, LLNL researchers Tom Guilderson and Stewart Fallon used radiocarbon dating to determine the ages of gold coral and deep-water black coral. The longest lived in both species was 2,740 years and 4,270 years old, respectively. At more than 4,000 years old, the deep-water black coral is the oldest living skeletal-accreting marine organism known. "And to the best of our knowledge, the oldest colonial organism yet found," Guilderson said. "Based on the carbon-14, the living polyps are only a few years old, or at least their carbon is, but they have been continuously replaced for centuries to millennia while accreting their underlying skeleton." The research appeared in the March 23 early online edition of the ***Proceedings of the National Academy of Sciences***.

Using a manned deep-sea research submersible, the team used samples that were individually



A deep-sea research submersible is used to retrieve the samples.

collected from the Makapuu and Lanikai deep-sea coral beds off the coast of Oahu, Keahole Point deep-sea coral bed off the coast of the Big Island and Cross Seamount about 100 miles south of Oahu. Carbon dating uses radiocarbon (carbon-14) to date the age of an object. Radiocarbon is the most widely used geochronological tool in the earth sciences for the late Quaternary (the last 50,000 years). Earlier radiocarbon studies showed that individual gold coral colonies from the Atlantic and Pacific oceans have life spans of 1,800 to 2,740 years, but the results remain contentious with some biologists. In particular, some have questioned whether the corals feed on re-suspended sediment (which could be old) and not on recently photosynthesized carbon that falls through the water column, or that they grew faster and then stopped growing when they reached a certain size. To answer these questions, the group analyzed not only polyps (the living animals that make up corals) but a branch of one specimen. The living animals had the same carbon-14 concentration as the overlying surface water. This shows that the carbon in the polyps was recently photosynthesized in the surface prior to being "eaten" by the polyps. The skeleton's carbon-14 concentration mimicked that of the overlying surface water's "post-bomb" time series: the time since the late 1950s when the testing of nuclear weapons augmented the natural abundance of carbon-14 in the atmosphere.

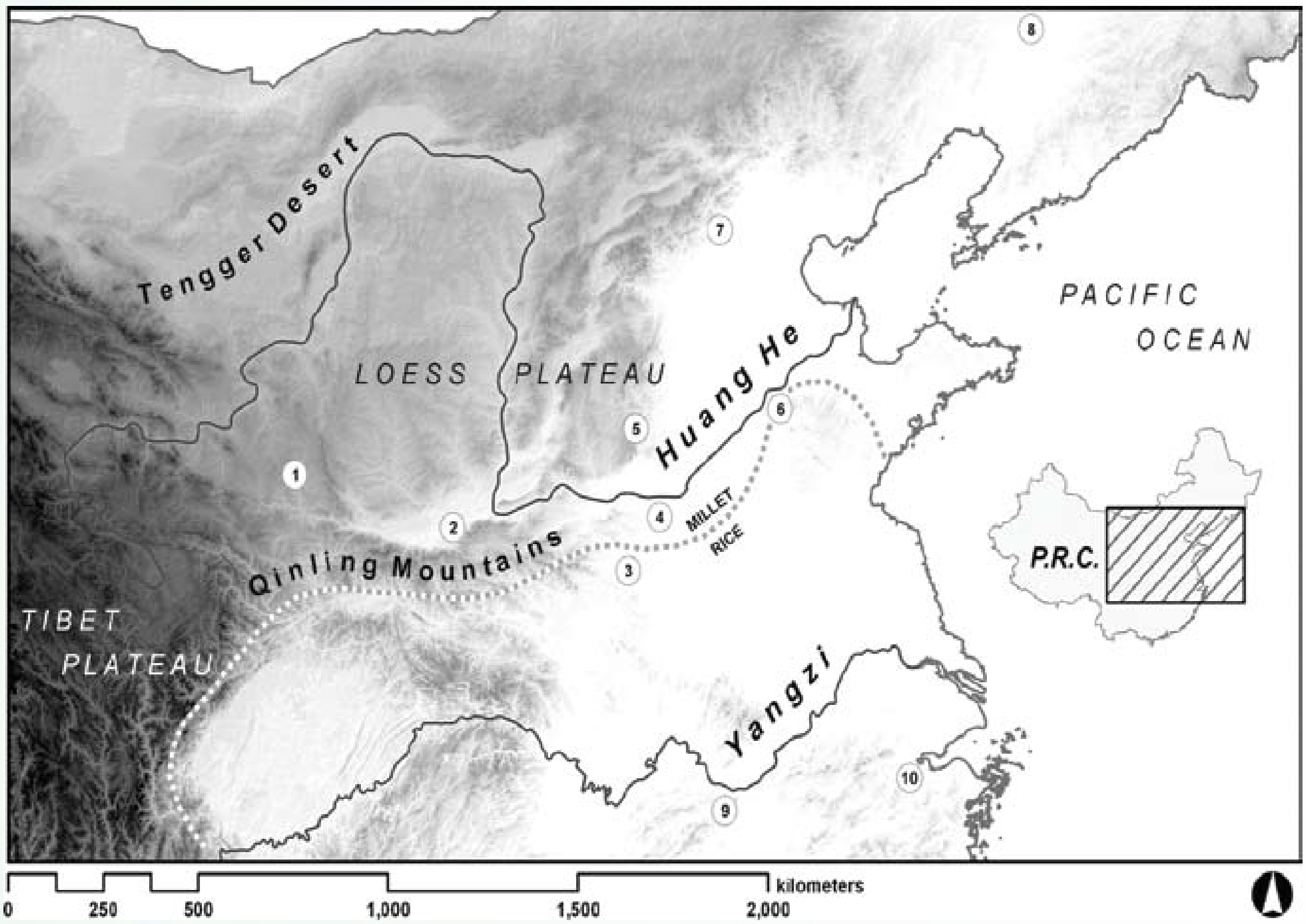
The radial growth rate during the last 50 years is similar to the long-term growth rate of the 300-year branch. The radial growth rate also is consistent with that derived from larger fossil samples. The radial growth rate is similar within a rather small range of tens of micrometers per year for all specimens analyzed. In the recent research, the Geradia coral was assumed to be much younger when amino acid and growth band methods were used. With radiocarbon dating, the average life span of the analyzed specimens is 970 years and ranges from about 300 years for a small branch (with a radius of 11 millimeters) to about 2,700 years (with a radius of 38 mm). "These ages indicate a longevity that far exceeds previous estimates," Guilderson said. "Many of the Geradia samples that we have analyzed are branches, not the largest portions of the colony and so the ages may not indicate how old the entire individual is." Hawaiian deep sea corals face direct threats from harvesting for jewelry and from commercial fisheries that trawl the ocean bottoms. In addition, the close relationship between deep-sea corals (and the mid-water ecosystems) and ocean's surface means that they can be affected by natural and man-made changes in surface ocean conditions, including ocean acidification, warming and altered stratification. The antiquity of the coral is an additional call for action, Guilderson said. "The extremely long life spans reinforce the need for further protection of deep-sea habitat" he said. "The research has already had an impact for activities in Hawaiian waters where a harvesting and fishing moratorium has been enacted to protect certain areas. There are similar habitats in international waters and it is hoped that the results will provide the scientific basis for agreements under the Law of the Sea, and United Nations Environment Programme."

Contact: Tom Guilderson (925) 422-1753 (guilderson1@llnl.gov)

Results give insight on earliest animal domestication

Tom Guilderson, of AEED, was part of a team using stable isotope and radiocarbon dating of ancient human and animal bone to document two distinct phases of plant and animal domestication in northwest China (see map). The dating work—conducted at PLS's Center for Accelerator Mass Spectrometry and published in the ***Proceedings of the National Academy of Sciences*** on March 23, 2009—has added new insight to detecting the symbiotic human–plant–animal linkages that developed during the very earliest phases of domestication. In the first phase—between 7,900 and 7,200 years ago—people harvested and stored enough broomcorn millet to feed themselves and their hunting dogs throughout the year. In the second, much more intensive phase, which was in place by 5,900 years ago, two different food sources—millet and rice—were cultivated and made significant contributions to the diets of people, dogs, and pigs. The stable isotope methodology used in this work is helping to explain how and why agriculture began in East Asia.

Contact: Tom Guilderson (925) 422-1753 (guilderson1@llnl.gov)



Climate models confirm more moisture in atmosphere attributed to humans

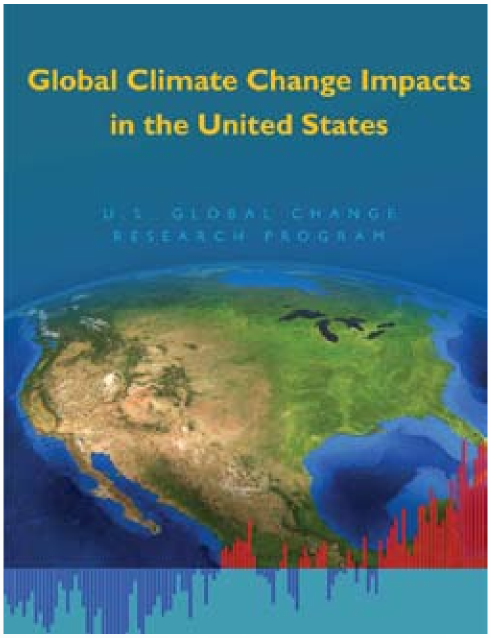
When it comes to using climate models to assess the causes of the increased amount of moisture in the atmosphere, it doesn't much matter if one model is better than the other. They all come to the same conclusion: Humans are warming the planet, and this warming is increasing the amount of water vapor in the atmosphere. In new research appearing in the August 10 online issue of the ***Proceedings of the U.S. National Academy of Sciences***, Livermore scientists and a group of international researchers found that model quality does not affect the ability to identify human effects on atmospheric water vapor. "Climate model quality didn't make much of a difference," said Benjamin Santer, lead author from LLNL's Program for Climate Modeling and Intercomparison. "Even with the computer models that performed relatively poorly, we could still identify a human effect on climate. It was a bit surprising. The physics that drive changes in water vapor are very simple and are reasonably well portrayed in all climate models, bad or good." The atmosphere's water vapor content has increased by about 0.4 kilograms per square meter per decade since 1988, and natural variability alone can't explain this moisture change, according to Santer. "The most plausible explanation is that it's due to human-caused increases in greenhouse gases," he said. More water vapor—which is itself a greenhouse gas—amplifies the warming effect of increased atmospheric levels of carbon dioxide.

Previous LLNL research had shown that human-induced warming of the planet has a pronounced effect on the atmosphere's total moisture content. In that study, the researchers had used 22 different computer models to identify a human "fingerprint" pattern in satellite measurements of water vapor changes. Each model contributed equally in the fingerprint analysis. "It was a true model democracy," Santer said. "One model, one vote." But in the recent study, the scientists first took each model and tested it individually, calculating 70 different measures of model performance. These "metrics" provided insights into how well the models simulated today's average climate and its seasonal changes, as well as on the size and geographical patterns of climate variability. This information was used to divide the original 22 models into various sets of "top ten" and "bottom ten" models. "When we tried to come up with a David Letterman–type 'top ten' list of models," Santer said, "we found that it's extremely difficult to do this in practice, because each model has its own individual strengths and weaknesses." Then the group repeated their fingerprint analysis, but now using only "top ten" or "bottom ten" models rather than the full 22 models. They did this more than 100 times, grading and ranking the models in many different ways. In every case, a water vapor fingerprint arising from human influences could be clearly identified in the satellite data. "One criticism of our first study was that we were only able to find a human fingerprint because we included inferior models in our analysis," said Karl Taylor, another LLNL co-author. "We've now shown that whether we use the best or the worst models, they don't have much impact on our ability to identify a human effect on water vapor."

This new study links LLNL's "fingerprint" research with its long-standing work in assessing climate model quality. It tackles the general question of how to make best use of the information from a large collection of models, which often perform very differently in reproducing key aspects of present-day climate. This question is not only relevant for fingerprint studies of the causes of recent climate change. It is also important because different climate models show different levels of future warming. Scientists and policymakers are now asking whether we should use model quality information to weight these different model projections of future climate change. "The issue of how we are going to deal with models of very different quality will probably become much more important in the next few years, when we look at the wide range of models that are going to be used in the Fifth Assessment Report of the Intergovernmental Panel on Climate Change," Santer said. Other LLNL researchers include Karl Taylor, Peter Gleckler, Celine Bonfils, and Steve Klein. Other scientists contributing to the report include Tim Barnett and David Pierce from the Scripps Institution of Oceanography; Tom Wigley of the National Center for Atmospheric Research; Carl Mears and

Frank Wentz of Remote Sensing Systems; Wolfgang Brüggemann of the Universität Hamburg; Nathan Gillett of the Canadian Centre for Climate Modelling and Analysis; Susan Solomon of the National Oceanic and Atmospheric Administration; Peter Stott of the Hadley Centre; and Mike Wehner of Lawrence Berkeley National Laboratory. The researchers' paper was also highlighted as an "Editor's Choice" by ***Science*** magazine. The comment, titled "Believable Fingerprints," notes that the "one model–one vote" method of predicting climate change "may not always be appropriate, even though it turned out that way in this study."

Contact: Ben Santer (925) 422-3840 (santer1@llnl.gov).



Report assesses impacts of climate change

Global warming is already occurring in the United States and the choices Americans make today will determine the severity of its impact in the future, according to a new report released on June 16, 2009. Report researchers representing 13 U.S. government science agencies, major universities and research institutes, including LLNL, produced the study entitled ***Global Climate Change Impacts in the United States***. Benjamin Santer of LLNL's Program for Climate Model Diagnosis and Intercomparison was a lead author of the first chapter, "Global Climate Change." "This part of the report explains why climate is changing and how we know that we are the ones causing it," Santer said. "Climate change is telling us a consistent story: Humans have had a pronounced effect on global climate." The most comprehensive report to date on the likely national impact of global climate change provides current information on changes in temperatures, rainfall patterns and sea level, and also focuses on the regional and sectoral effects of these changes. The study finds that Americans are already being influenced by climate change through extreme weather, drought and wildfire, and details how the nation's transportation, agriculture, health, water, and energy sectors will be affected in the future.

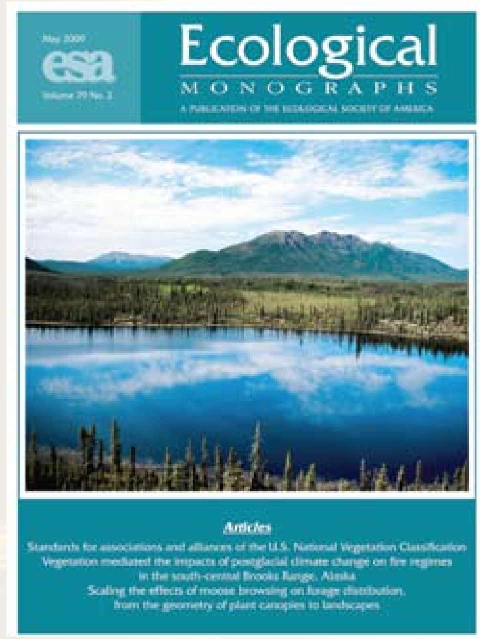
The study also finds that the current trend in the emission of greenhouse gas pollution is significantly above the worst-case scenario examined in this report. Santer's chapter finds that human activities have led to large increases in heat-trapping gases over the past century; global average temperature and sea level have increased, and precipitation patterns have changed; the global warming of the past 50 years is due primarily to human-induced increases in heat-trapping gases; and global temperatures are projected to continue to rise over this century—by how much and for how long depend on a number of factors, including the amount of heat-trapping gas emissions and how sensitive the climate is to those emissions. The emissions responsible for human-induced warming come primarily from the burning of fossil fuels (coal, oil, and gas) with additional contributions from the clearing of forests and agricultural activities. Global average temperature has risen by about 1.5° Fahrenheit since 1900. By 2100, it is projected to rise another 2° to 10° Fahrenheit. Increases at the lower end of this range are more likely if global heat-trapping gas emissions are cut substantially. If emissions continue to rise at or near current rates, temperature increases are more likely to be near the upper end of the range.

A product of the interagency U.S. Global Change Research Program and led by NOAA, the definitive 190-page report is written in plain language, intended to better inform members of the public and policymakers. It was commissioned in 2007. "Our report underscores the importance of reducing heat-trapping emissions by comparing impacts that will result from higher versus lower emissions," said Tom Karl, director of NOAA's National Climatic Data Center in Asheville, NC and one of the co-chairs of the report. "It shows that the choices made now will have far-reaching consequences." The report draws from a large body of scientific information, including the set of 21 Synthesis and Assessment reports from the U.S. Global Change Research Program. The government agencies affiliated with the program include the Departments of Agriculture, Commerce, Defense, Energy, Health and Human Services, Interior, State, and Transportation; the Environmental Protection Agency; NASA; National Science Foundation; Smithsonian Institution; and the United States Agency for International Development.

Contact: Ben Santer (925) 422-3840 (santer1@llnl.gov)

Plants' effect on wildfires elucidated

Rising temperatures may lead to more tinder-dry vegetation, but that doesn't mean there will be a higher risk for wildfires in a particular area—it all depends on the type of vegetation in the area. A new study on the cover of the May 2009 issue of ***Ecological Monographs*** shows that, in some cases, the types of plants growing in an area could override the effects of climate change on wildfire occurrence. AEED scientist Tom Brown, along with Philip Higuera of Montana State University and colleagues, looked at the direct and indirect impacts of millennial scale climate change on fire occurrence in the south-central Brooks Range in Alaska. The team looked at historical fire occurrence by analyzing sediments found in the bottom of lakes. Using the Lab's Center for Accelerator Mass Spectrometry, operated by PLS, they carbon-dated the deposits in the sediment, then measured the amount of charcoal in the sediments and reconstructed fire occurrences from 15,000 B.C. to the present. Finally they measured the amount of plant parts, such as fossil pollen, to figure out what type of vegetation dominated the area during the different time periods.



Like rings in a tree, different layers of sediment represent different times in the past. The conclusion: historical changes in fire frequencies coincided with changes in the type of vegetation in the area, more so than to rising temperatures alone. "If all we did was look at rising temperatures and ignore the vegetation in the area, that wouldn't be a good predictor of the likelihood of wildfires in a particular region," Brown said. "You have to look at the whole picture." Although changing temperatures and moisture content set the stage for changes in wildfire frequency, they can often be trumped by changes in the distribution and abundance of plants. Earlier studies have suggested that the area burned across arctic and boreal regions will increase over the next century as climate change lengthens the fire season, decreases moisture, and increases ignition rates. However, vegetation can alter the direct link between climate and fire by influencing the abundance, structure, and moisture content of fuels across space and time. "There's a complex relationship between fuels and climate," Brown said. "Vegetation can have a profound impact on fire occurrences that are opposite or independent of climate's direct influence on fire." In the recent study, the researchers found that changes in climate were less important than changes in vegetation. Despite a transition from a cool, dry climate to a warm, dry climate about 10,500 years ago, the researchers found a sharp decline in the frequency of fires. Their sediment cores from that time period revealed a vegetation change from flammable shrubs to fire-resistant deciduous trees.

"In this case, a warmer climate was likely more favorable for fire occurrence, but the development of deciduous trees on the landscape offset this direct climatic effect," Higuera said. The research implies that the impacts of climate change on modern-day fire frequencies could be strongly mediated by changes in vegetation. Thus, in some cases, the impacts of climate change on fire may be less intuitive than initially perceived. "This could give fire managers a good indication that vegetation can substantially alter the direct effects of climate change on fire occurrence," Brown said. Other contributors include the University of Washington and the University of Illinois-Urbana.

Contact: Tom Brown (925) 423-8507 (brown92@llnl.gov)

Tropical forest seed banks shown to reveal the past

Seeds of some tree species in the Panamanian tropical forest can survive for more than 30 years before germinating. That is 10 times longer than most field botanists had believed. Using the Lab's Center for Accelerator Mass Spectrometry to measure the amount of carbon-14 in seeds of the trees *Croton billbergianus, Trema micrantha, and Zanthoxylum ekmannii,* LLNL scientist Tom Brown and University of Illinois at Urbana-Champaign colleague James Dalling found that seeds survived in the soil for 38, 31, and 18 years, respectively. Previous demographic studies of pioneer tree species showed that seed persistence is short, lasting only for a few years at most. But in the tropical forests of Barro Colorado Island, Panama, Brown and Dalling found the seeds of some pioneer trees remain viable for many years. "This is part of nature that wasn't really what people in the field thought was going on," Brown said. "It turns out these seeds in soil just a few centimeters below the surface can survive a lot longer than anyone ever thought was possible."

To increase the probability of encountering "old" seeds, Brown and Dalling used data from a forest plot to target sites in the forest occupied 20 years previously by species they suspected were capable of long-term persistence. After Dalling germinated seeds extracting from surface soil layers at these sites, Brown carbon-dated samples taken from the seed coat. However, unlike carbon dating techniques used by archaeologists to estimate the age of objects from antiquity, he used a modern radiocarbon signal that is a consequence of atmospheric nuclear testing in the 1950s and early 1960s. The decline in radiocarbon concentration that has occurred since the test-ban treaty went into effect can be used as a signal to determine precisely when carbon became incorporated into plant tissue. When disturbance kills canopy trees in tropical forest, light reaches the forest floor, triggering the germination of seeds of pioneer tree species buried in the soil. The age of these seeds, and thus the time that populations of pioneer species are able to survive between disturbance events, has long been open to question. "This is a surprising result," Dalling said. "Demographic

A canopy of trees in the tropical forests of Barro Colorado Island, Panama.

models suggest that these species would not benefit from long persistence, and we doubted they would be able to survive anyway. Seeds dispersed onto the soil surface are prey to insect seed predators, and are exposed to an array of pathogens and decay organisms that proliferate in moist tropical soils." The results imply that buried seeds may be an important reservoir for genetic diversity in pioneer populations and may be as important as long-distance dispersal in maintaining populations in fragmented habitats. The research appears in the April edition of ***The American Naturalist.***

Contact: Tom Brown (925) 423-8507 (brown92@llnl.gov)

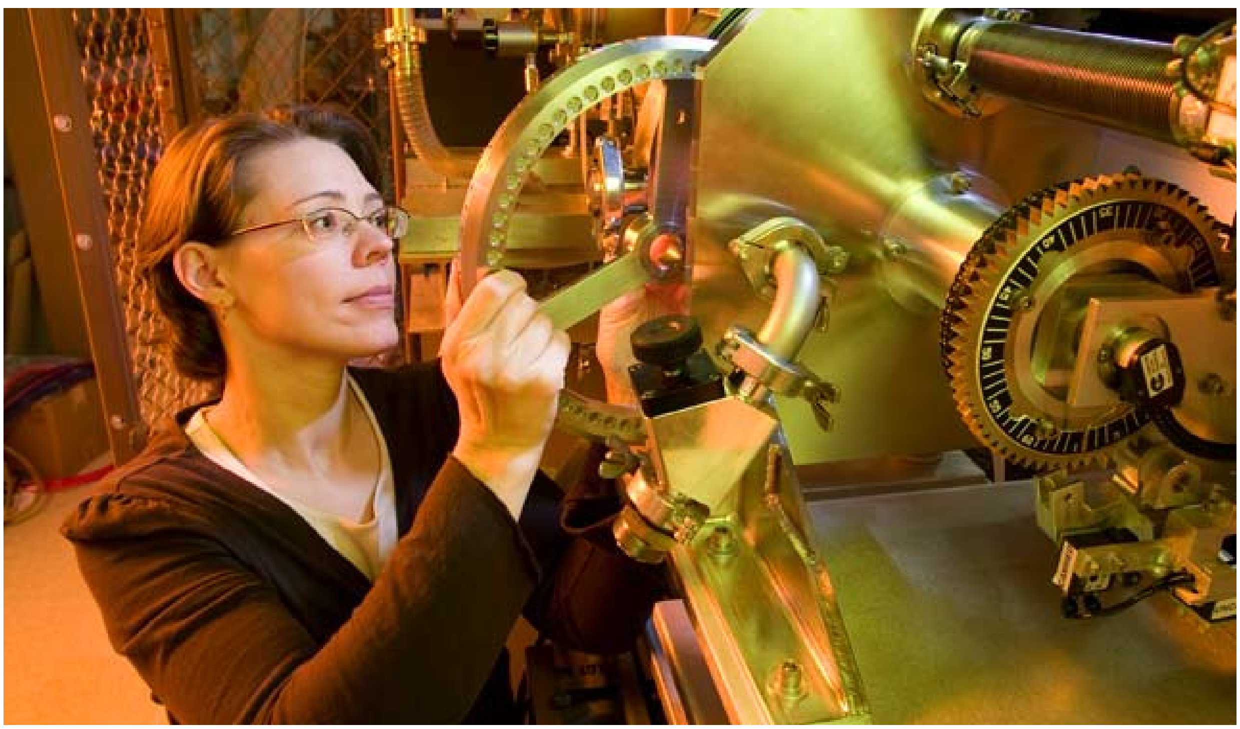
Investigating California's climate record

As part of the Laboratory's efforts to predict future climate change, AEED researcher Susan Zimmerman is spearheading a project to develop high-precision paleoclimate records for use in regional climate models. Current models typically use data for only the last 150 years and, thus, miss wet and dry periods from past millennia.

"Remarkably, over the last century, the West has been relatively wet compared to the average for the last 2,000 years," says Zimmerman. "Without more long-term data, predictive modeling is biased toward these anomalously wet conditions."

Zimmerman is working with researchers across California to analyze lake sediments and develop records that span the last two millennia. "Lakes are long-lived, wet areas where materials are continually deposited over time," she says. Data from these records will be used to map previous drought patterns in California and help climate modelers more accurately simulate the range of natural climate changes. With this information, state agencies can determine the infrastructure needed to meet future demands for water.

She and her collaborators collect samples from natural outcrops such as stream cuts or from vertical cores of sediment extracted from a basin. Layers in the core indicate the conditions under which the sediment was deposited. Zimmerman analyzes samples at the Laboratory's Center for Accelerator Mass Spectrometry, where she works with Livermore scientists Tom Guilderson, Tom Brown, and Graham Bench. Zimmerman



Susan Zimmerman loads a sample wheel into the ion source of an accelerator mass spectrometer.

pretreats each sample, which may be charcoal, pine needles, or other macrofossils; combusts it into carbon dioxide gas; and then catalyzes the gas into graphite powder. The powder is pounded into aluminum sample targets, which are arranged with standard targets and blanks in a sample wheel and loaded into the spectrometer. With the high-precision accelerator mass spectrometer, Zimmerman can determine a sample's radiocarbon age to within 20 years.

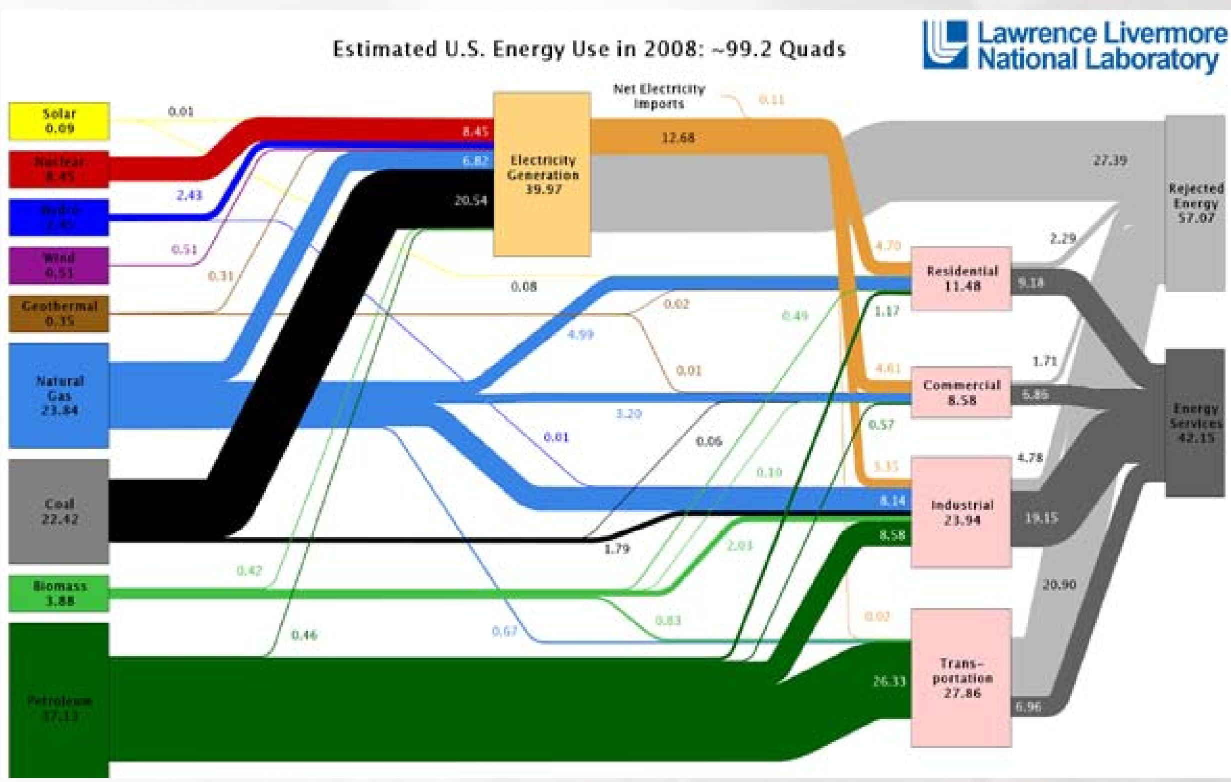
Once the radiocarbon dates are calibrated to calendar years, Zimmerman and her colleagues establish a chronology for the paleoclimate records from the original core or outcrop. These records are then compared to other sources of ancient climate information, such as tree rings, to develop a regional picture. Combining well-dated paleoclimate records from statewide sites, Zimmerman will create time-slice maps of wet and dry patterns in California in 100-year intervals. In the last phase of her project, she will analyze spectra of the paleoclimate records to look for influences from mechanisms such as the El Niño climate pattern and the Pacific Decadal Oscillation, a long-term surface fluctuation of the Pacific Ocean.

"The Laboratory offers me the opportunity to work with many people in my field," says Zimmerman. This relationship with colleagues benefits everyone involved. Not only does Zimmerman get to do field work in new places and handle a variety of samples, but she also provides researchers statewide with data that might otherwise not be available to them. In addition, the data collected in her project will help strengthen the Laboratory's climate model predictions. With improved models, decision makers can better prepare for what research indicates will be a drier California in the next several decades.

Contact: Susan Zimmerman (925) 422-8462 (zimmerman17@llnl.gov)

Distilling the big picture about energy resources into a concise diagram

LLNL produced the first diagrams illustrating U.S. energy use in the mid-1970s. Portraying U.S. energy resources and their ultimate use, these diagrams, called energy flow charts, help scientists, analysts, and other decision makers to visualize the complex interrelationships involved in powering the nation.



The 2008 chart (available online at publicaffairs.llnl.gov/news/energy/energy.html) shows that U.S. energy usage dropped from 101.5 quadrillion British thermal units, or quads, in 2007 to 99.2 quads in 2008.

The charts continue to provide value, drawing widespread attention and praise from such organizations as the National Academy of Sciences and the President's Council of Advisors on Science and Technology.

Nalu Kaahaaina, deputy project director for Energy and Environmental Security in the Global Security Principal Directorate, has overall responsibility for Livermore's development of the energy flow charts, and engineer A. J. Simon, of PLS's AEED, leads the analysis. The researchers, both previously lecturers at Stanford University, note that the Laboratory's work on the energy diagrams is one reason they chose to come to Livermore. "A huge community of experts is performing energy systems analysis," says Simon, "but Livermore is one of the few organizations that distills 'the big picture' into a concise visual representation." Because the Laboratory's staff includes a variety of experts working across disciplines, it is uniquely qualified to develop the charts.

Simon has already harnessed Laboratory expertise in algorithm design, physics-based modeling, and system analysis to produce increasingly refined assessments of U.S. energy resources and consumption. "Originally, producing these charts required a member of our technical staff to review an EIA report and a graphics designer to produce the image," says Simon. "Now, we automate the routine data synthesis with a software engine that renders the image." Instead of having a person read through a 400-page report, the analysis tool calculates a set of intermediates, ultimately generating approximately 30 energy statistics. This greatly speeds the process—which once took a week—enabling the analyst to now spend a few hours interpreting the results after only a few seconds of processing.

"The relative simplicity of the diagrams sometimes belies the initial effort to build them," says Simon. "Ultimately, this effort is about taking complex systems and sharing them with broader audiences. The less daunting the information is, the more impact it can have. Simplicity is a compliment."

Energy informatics will improve the methods available for visualizing these types of data. As a result, says Simon, "we will be better able to answer the questions we receive from other researchers, and we can develop more useful products for a variety of users." The team is currently searching for a sponsor to support an energy informatics program at the Laboratory.

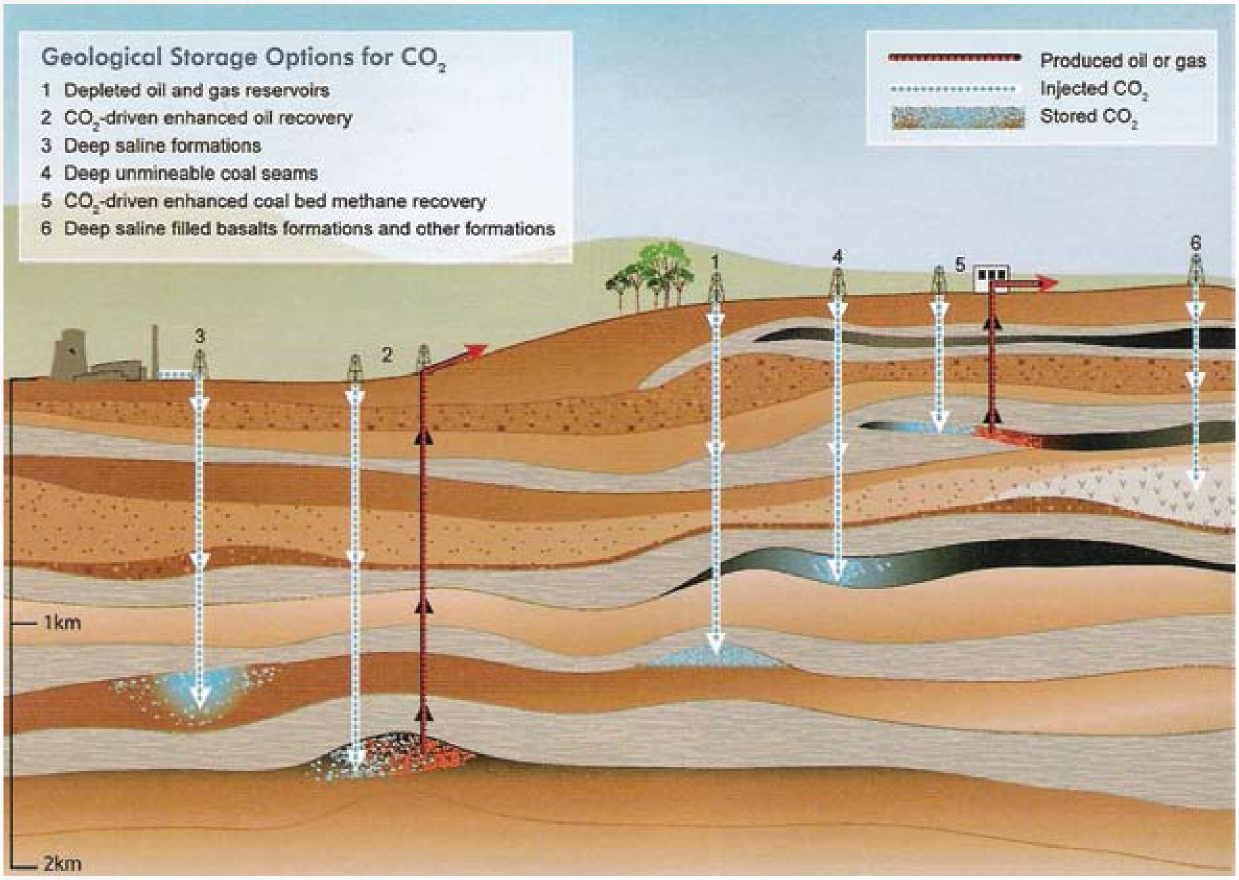
For Livermore's mission-related work on energy and environmental security, the flow charts are an ideal tool to analyze not only energy but also carbon, water, and other relevant "networks." One chart portrays the estimated carbon dioxide emissions associated with all energy resources. Such analyses provide insights that simultaneously enable system optimization, for example, identifying underused resources or the need for better technology, and reveal cross-system couplings, such as carbon embedded in energy or water demand for electricity generation.

Contact: A. J. Simon (925) 422-9862 (simon19@llnl.gov)

Underground testing for carbon sequestration

The Big Sky Carbon Sequestration Partnership consists of universities, national laboratories, private companies, state agencies, and Native American tribes and encompasses Montana, Wyoming, Idaho, South Dakota, and eastern Washington and Oregon. The project relies on existing technologies from the fields of engineering, geology, chemistry, biology, geographic information systems, and economics to develop new approaches for geologic carbon storage in the region. Appropriate geological formations for carbon storage have a caprock overlaying an impermeable rock layer that prevents the CO_2 from returning to the atmosphere. The CO_2 is injected at a rate slow enough so that it can dissipate throughout the rock. Geological formations well suited for carbon storage include deep saline formations, flood basalt formations, depleted oil and gas reserves, and unmineable coal beds. The Big Sky program focuses on large saline aquifers in Montana and Wyoming.

The next phase of the Big Sky project is under way with a pilot sequestration project in southeast



Geological sequestration is the process of capturing CO from point-sources, such as a power plant, and storing it permanently in deep underground geological formations. CO_2 can be stored in deep saline formations, flood basalt formations, oil and gas reservoirs, and unmineable coal seams.

Washington in which 1,000 tons of carbon will be stored deep in a basalt formation. Big Sky Outreach and Community Coordinator Lindsey Waggoner said Phase II is designed to validate the technical and economic feasibility of carbon sequestration, develop monitoring and verification protocols, and analyze the policy and regulatory frameworks of carbon sequestration in the Big Sky region.

Phase III of the project will involve a demonstration project in an existing natural gas processing facility in Wyoming in which the natural gas and CO_2 are already separated. The CO_2 will be pushed more than 10,000 feet deep into a large saline aquifer close to the plant.

Contact: Roger Aines (925) 423-7184 (aines1@llnl.gov)

Postdoc analyzes North Korean seismic event

Sean Ford, a postdoctoral researcher in AEED, is the first author on a paper—"Source analysis of the Memorial Day explosion, Kimchaek, North Korea"—written with co-authors Doug Dreger of UC Berkeley and Bill Walter of PLS and published in the November 7 issue of ***Geophysical Research Letters***. The authors used full-waveform analysis to characterize the alleged nuclear explosion in North Korea in May of 2009 and showed that an earthquake source is inconsistent with the data. Future analyses of this type could be used to identify and characterize non-earthquake events such as explosions and mine collapses.

Contact: Sean Ford (925) 424-6998 (ford17@llnl.gov)

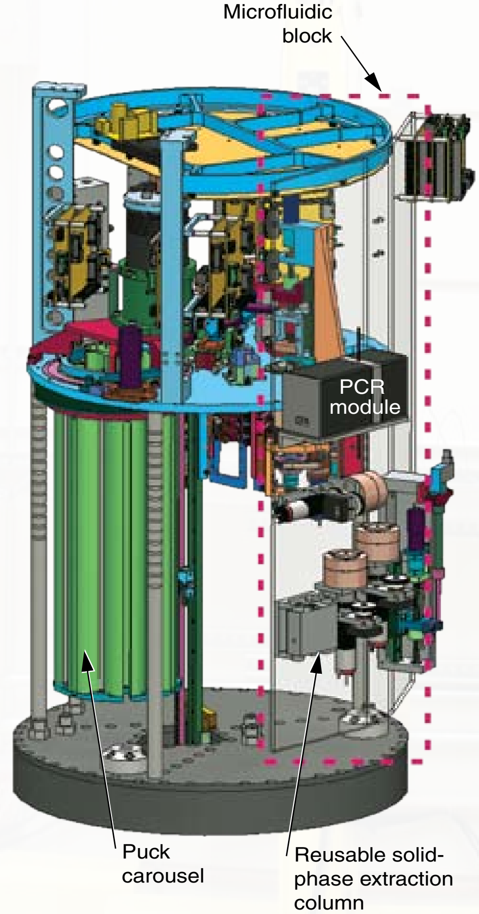
Life Sciences

DNA analysis technology to discover new marine species and prepare to search for life on other planets

The Monterey Bay Aquarium Research Institute (MBARI), a nonprofit organization in Moss Landing, CA, is one of several institutions developing instruments to aid the search for aquatic life forms and to further scientific research on microbes' role in mediating the cycling of Earth's elements and energy. Livermore scientists and engineers have joined the MBARI search for new life forms by designing an autonomous electro-opto-mechanical device that detects microbial genes of interest and measures their preponderance. The device, a polymerase chain reaction (PCR) module, incorporates features from Livermore-designed systems that detect pathogens, but it is much more compact and "intelligent" than previous instruments.

Data produced by the PCR module will help researchers better understand the roles microbes may play in responding to global climate change. By studying the genetic makeup of these species, scientists can learn how microbes remove carbon from the atmosphere and cope with the increasing acidity of oceans. By any measure, one of Earth's extreme environments is the deep sea, where superheated (more than 350°C) fluids mix with near-freezing seawater at several hundred atmospheres of pressure, where 1 atmosphere equals more than 100 kilopascals. Compared to most of the deep sea, the areas immediately around hydrothermal vents typically support complex microbial communities. Deep-sea studies may also contribute to astrophysics research because extreme environments on Earth could be similar to conditions elsewhere in the solar system. For example, the surface of Europa (a Jupiter satellite) appears to be entirely submerged beneath a sea covered with thick ice. Some scientists speculate that primitive life forms resembling Earth's microbes could exist around active volcanoes or hydrothermal vents believed to exist on Europa's seafloor.

To analyze marine organisms in their native habitats, MBARI scientists developed the Environmental Sample Processor (ESP). This remote instrument system collects water samples and puts them through several stages of filtration to obtain a variety of microbes. The processor lyses, or bursts, the filtered cells, releasing DNA, RNA, and proteins. It then forwards concentrated extracts to instruments that analyze the genetic material and identify the microbes and their gene products, such as deadly marine toxins. ESP also archives samples for further analysis after the device is recovered and returned to land. Livermore's PCR module is a stand-alone system that provides enhanced analysis downstream of routine sample-processing operations.



This model shows the core ESP with a PCR module and microfluidic block attached on the right-hand side.

After concluding that PCR would be the optimal technique for them, MBARI turned to Livermore researchers to design the compact PCR module because of their expertise with this technology. Over the past decade, the Laboratory has developed a number of PCR-based systems that rapidly detect and identify airborne and other environmental biological agents. Among such systems are the handheld advanced nucleic acid analyzer and the autonomous pathogen detection system (APDS). APDS monitors the air for biological threat agents including bacteria, viruses, and toxins, and units can operate continuously in public areas such as subway stations.

"Our challenge was to develop a compact, low-power, smart system to run PCR reactions and take measurements," says Livermore chemical and mechanical engineer John Dzenitis, who led the PCR module development effort. "Running PCR underwater had never been done before. We were confident we could do it, though, because operating the sample processor is analogous to running an APDS unit underwater. Before we developed APDS, no one had autonomously operated this type of detector in a subway."

The performance goals for the PCR module were similar to those for an APDS unit, but the underwater device had to be self-contained. In addition, the Livermore team wanted to provide fast heating and cooling cycles and at least two optical channels for reading concentrations of different fluorescent-labeled molecules. The team also had to ensure that the device drew minimal power from ESP's marine batteries and interfaced seamlessly with the processor's fluid-shuttling systems. Finally, the module had to be easy to program and able to function without receiving external commands.

Although the PCR module can be used on all ESPs, it was designed with Deep ESP in mind. This version of the processor, which can operate in waters as deep as 4,000 meters, includes an original ESP surrounded by a 1-centimeter-thick titanium pressure housing. Deep ESP can be placed on the sea bottom and hooked to a cable carrying power and data from shore or a buoy and linked by satellite to researchers on shore. MBARI researchers ran the first samples through a Deep ESP in May 2009.

Scientists are especially interested in using Deep ESP to study organisms that have evolved over millions of years to survive in such extreme environments as the methane seeps in the Santa Barbara Basin or the hot, deep-sea vents found at the Axial Seamount submarine volcano off the Oregon coast. The MBARI team conducted a Deep ESP expedition near the Axial Seamount in 2009 to study the interaction between volcanic events and thriving microbial populations. Another potential environment to study is an area adjacent to methane hydrate ("fire ice") outcroppings off California, Oregon, and Washington. These outcroppings, which consist of methane trapped within ice, support large microbial populations.

The Livermore team delivered the first PCR module to MBARI in 2007 and additional units for further testing in 2008 and 2009.

Contact John Dzenitis (925) 422-6695 (dzenitis2@llnl.gov)

Paper highlighted in *Nature Chemical Biology*

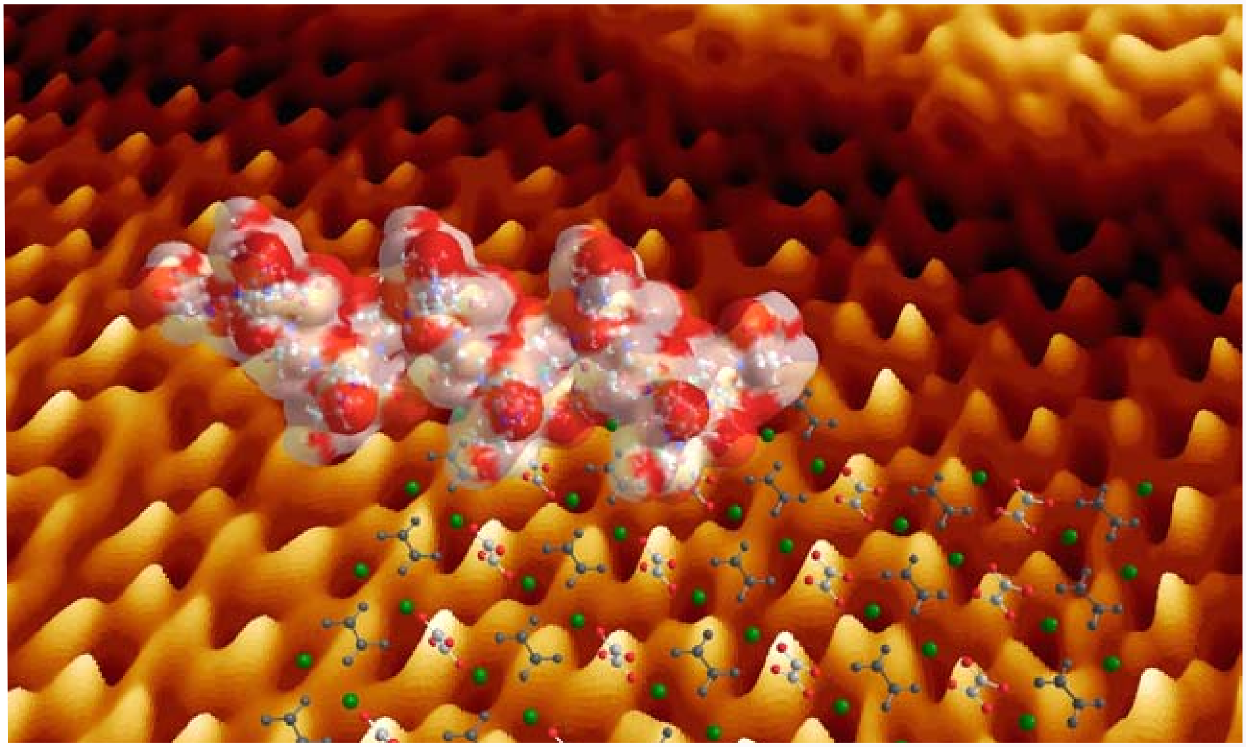
A paper by Ali Navid and Elvind Almass—"Genome-scale reconstruction of the metabolic network in *Yersinia pestis* strain 91001"—was published in the ***Molecular BioSystems Journal*** and was also highlighted by ***Nature Chemical Biology***, which stated:

> *Yersinia pestis*, the causative agent of the bubonic plague, remains a modern concern. There is no vaccine for this deadly bacterium, and resistance may be on the rise. Direct experimentation with the organism is limited to high-security labs, so alternate methods to gain insights into the complex workings of these cells are urgently needed. Flux-balance analysis (FBA) has been used to create genome-scale models of metabolism by identifying metabolic network structure and steady state activity patterns. Navid and Almaas now use this technique with *Y. pestis,* creating an initial model containing 1,020 enzymatic reactions and 825 metabolites. However, their analysis was complicated by the fact that the organism is meiotrophic, meaning that it contains cryptic genes that are silent unless activated under certain conditions. In order to overcome this obstacles they have developed a new computational tool called "CryptFind," which utilizes constraint-based modeling to identify the set of candidate cryptic genes that are responsible for the meiotrophic behavior.

Contact: Ali Navid (925) 424-3564 (navid1@llnl.gov)

Scientists see peptides control crystal growth with "switches, throttles and brakes"

By producing some of the highest resolution images of peptides attaching to mineral surfaces, scientists have a deeper understanding how biomolecules manipulate the shape of growing crystals. The research, which appeared in the January 2010 issue of the ***Proceedings of the National Academy of Science***, explores how peptides interact with mineral surfaces by accelerating, switching and inhibiting their growth. The team—made up of researchers from LLNL (S. Roger Qiu), the Molecular Foundry at Lawrence Berkeley (Raymond W. Friddle and James J. De Yoreo), the University of California, Davis (Matthew L. Weaver and William H. Casey) and the University of Alabama (Andrzej Wierzbicki)—for the first time produced single-molecule resolution images of this peptide–mineral interaction. Inorganic minerals play an important role in most biological organisms. Bone, teeth, protective shells, or the intricate cell walls of marine diatoms are some displays of biomineralization, where living organisms form structures using inorganic material. Some minerals also can have negative effects on an organism such as in kidney and gallstones, which lead to severe suffering and internal damage in humans and other mammals. Understanding how organisms limit the growth of pathological inorganic minerals is important in developing new treatment strategies. But deciphering the complex pathways that organisms use to create strong and versatile structures from relatively simple materials is no easy feat. To better understand the process, scientists attempt to mimic them in the laboratory. By improving the resolution power of an Atomic Force Microscope (AFM), the PNAS authors were able to image individual atomic layers of the crystal interacting with small protein fragments, or peptides, as they fell on the surface of the crystal. "Imaging biomolecules that are weakly attached to a surface, while simultaneously achieving single-molecule resolution, is normally difficult to do without knocking the molecules off," said Raymond Friddle, a former LLNL postdoctoral fellow.



Aspartic acid-rich peptides adsorbed on a calcium oxalate monohydrate (COM) crystal surface. Models of a peptide and COM crystal structure are overlain on an AFM image collected during growth of the [010] face of COM. The rendered AFM image reveals the molecular structure of the crystal surface, including individual kink sites along a single atomic step.

The team, however, improved upon previous methods and achieved unprecedented resolution of the molecular structure of the crystal surface during the dynamic interaction of each growing layer with peptides. "We were able to watch peptides adhere to the surface, temporarily slow down a layer of the growing crystal, and surprisingly 'hop' to the next level of the crystal surface, says Friddle."

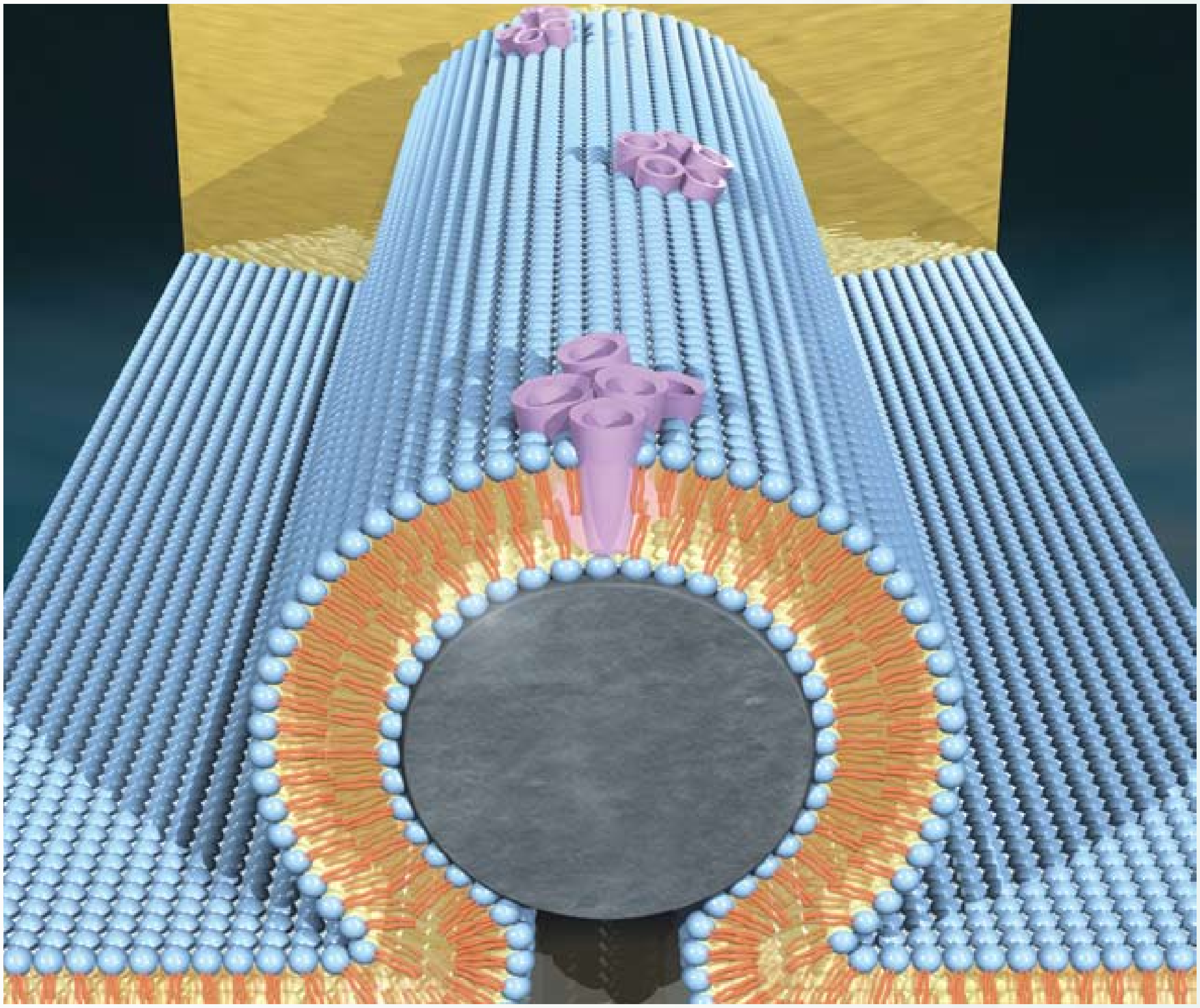
The images also revealed a mechanism that molecules can use to bind to surfaces that would normally repel them. The high-resolution images showed that peptides cluster together on crystal faces that present the same electronic charge. Under certain conditions the peptides would slow down growth, while under other conditions the peptides could speed up growth. On another face of the crystal, where the peptides were expected to bind strongly, the researchers found instead that the peptides did not attach to the surface unless the crystal growth slowed. The peptides needed to bind in a specific way to the face, which takes more time than a non-specific attachment. As a result, the growing layers of the crystal were able to shed off the peptides as they attempted to bind. But when the researchers slowed down the crystal growth rate, the peptides collapsed onto the surface so strongly that they completely stopped growth. The researchers proposed that the phenomenon is due to the unique properties of biopolymers, such as peptides or polyelectrolytes, which fluctuate in solution before resting in a stable configuration on a surface. "The results of the catastrophic drop in growth by peptides suggest ways that organisms achieve protection against pathological mineralization," said Jim De Yoreo (formerly of LLNL), the project lead and deputy director of research at LBNL's Molecular Foundry. "Once growth is halted, a very high concentration of the mineral will be needed before growth can again reach significant levels." He said designing polyelectrolyte modifiers in which the charge, size and ability to repel water can be systematically varied would allow researchers to create the equivalent of "switches, throttles and brakes" for directing crystallization.

Contact: S. Roger Qiu (925) 422-1636 (qiu2@llnl.gov)

Nanoelectronic transistor combined with biological machine could lead to better electronics

If man-made devices could be combined with biological machines, laptops and other electronic devices could get a boost in operating efficiency. Livermore researchers have devised a versatile hybrid platform that uses lipid-coated nanowires to build prototype bionanoelectronic devices. Inserting biological components in electronic circuits could enhance biosensing and diagnostic tools, advance neural prosthetics such as cochlear implants, and could even increase the efficiency of future computers. While modern communication devices rely on electric fields and currents to carry the flow of information, biological systems use a different signaling system: They use an arsenal of membrane receptors, channels and pumps to control signal transduction on a level that is unmatched by even the most powerful computers. For example, conversion of sound waves into nerve impulses is a very complicated process, yet the human ear has no trouble performing it. "Electronic circuits that use these complex biological components could become much more efficient," said Aleksandr Noy, lead scientist on the project. While earlier research has attempted to integrate biological systems with microelectronics, none have gotten to the point of seamless material-level incorporation. "But with the creation of even smaller nanomaterials that are comparable to the size of biological molecules, we can integrate the systems at an even more localized level," Noy said.

To create the bionanoelectronic platform the LLNL team turned to lipid membranes, which are ubiquitous in biological cells. These membranes form a stable, self-healing, virtually impenetrable barrier to ions and small molecules. "That's not to mention that these lipid membranes also can house an unlimited number of protein machines that perform a large number of critical recognition, transport and signal transduction functions in the cell," said Nipun Misra, a UC Berkeley graduate student and a co-author on the paper. Julio Martinez, a UC Davis graduate student and another co-author added: "Besides some preliminary work,



An artist's representation of a bio-anoelectronic device incorporating alamethicin biological pores. In the core of the device is a silicon nanowire (grey), covered with a lipid bilayer (blue). The bilayer incorporates bundles of alamethicin molecules (purple) that form pore channels in the membrane. Transport of protons through these pore channels changes the current through the nanowire.

using lipid membranes in nanoelectronic devices remains virtually untapped." The researchers incorporated lipid bilayer membranes into silicon nanowire transistors by covering the nanowire with a continuous lipid bilayer shell that forms a barrier between the nanowire surface and solution species. "This 'shielded wire' configuration allows us to use membrane pores as the only pathway for the ions to reach the nanowire," Noy said. "This is how we can use the nanowire device to monitor specific transport and also to control the membrane protein." The team showed that by changing the gate voltage of the device, they can open and close the membrane pore electronically. The research appeared on August 10 in the online version of the ***Proceedings of the National Academy of Sciences***.

Contact: Yinmin Wang (925) 422-6083 (wang35@llnl.gov)

Research reveals potential hope for heart attack victims

By using the amount of carbon-14 in the atmosphere from above-ground nuclear testing in the 1950s and 1960s, researchers have determined that cells in the human heart develop into adulthood. But as humans age, the percentage of new heart cells decreases markedly. By age 25, renewal of heart cells gradually decrease from 1 percent turning over annually to 0.45 percent by the age of 75. About 50 percent of the heart cells a human is born with will regenerate during a lifetime. Myocardial damage often results in chronic heart failure because of the loss and insufficient regeneration of heart cells.

This new finding, however, may mean that patients, who have suffered myocardial damage as a result of a heart attack, may have some good news. Lawrence Livermore's Bruce Buchholz, with colleagues from the Karolinska Institute, Université Claude Bernard Lyon, Lund University and Lund University Hospital, found that cells in a human heart can develop into adulthood and the age of heart cells is, on average, 6 years younger than the individual. Using the Laboratory's Center for Accelerator Mass Spectrometry, Buchholz measured the amount of carbon-14 in DNA to establish the age of caridiomyocytes (cardiac muscle cells) in humans. Carbon-14 atmospheric concentration levels remained relatively stable until the Cold War, when above-ground nuclear bomb tests caused a sharp increase, or peak, which decreased slowly after the end of above-ground testing in 1963. This spike in carbon-14 in the atmosphere serves as a chronometer of the past 55 years. Because DNA is stable after a cell has gone through its last cell division, the concentration of carbon-14 in DNA serves as a date mark for when a cell was born and can be used to date cells in humans. The team determined the ages of heart cells by determining the time at which the sample's carbon-14 concentration corresponded to the atmospheric concentration. Buchholz found that people born around or after the nuclear bomb tests corresponded to atmospheric concentrations several years after the subjects' birth, indicating substantial postnatal DNA syntheses. "By analyzing individuals born at different times before 1955, it is possible to establish the age up to which DNA synthesis occurs, or whether it continues beyond that age," Buchholz said.

In the study, carbon-14 concentrations were elevated in subjects compared to those people born up to 22 years before the beginning of nuclear bomb tests. "DNA of myocardial cells is synthesized many years after birth, indicating that cells in the human heart do, in fact, renew into adulthood," Buchholz said. "At the age of 50, 55 percent of the heart's cells remain from the time around birth and 45 percent have been generated later." Cardiac muscles have a striated appearance and their contraction in the heart propels blood from the atria and ventricles to the blood vessels of the circulatory system. The limited recovery in humans after a heart injury, such as a heart attack, demonstrates failing regeneration of heart cells. But the team concluded that the renewal of heart cells, as indicated by the mixing of carbon-14 in the DNA, suggest that the development of pharmacological strategies to stimulate this process may be a rational alternative or complement to cell transplantation strategies for heart cell replacement. The research appeared in the April 3, 2009 edition of *Science*.

Contact: Bruce Buchholz (925) 422-1739 (buchholz2@llnl.gov)

Paper describes biological applications of nanoarrays

With the Physics Division's Jane Bearinger as principal investigator and lead author, an LLNL team along with colleagues at Stanford University and the Swiss Federal Institutes of Technology at Zurich and Lausanne recently published a paper in the April 29, 2009 edition of ***Molecular & Cellular Proteomics***. The team demonstrated how fabricated nanoarrays, with controlled features as small as 200 nm, exhibit regularly ordered patterns and may be appropriate for the rapid and parallel proteomic screening of immobilized biomolecules, the study of protein–protein interactions, and biophysical and molecular biology studies involving spatially dictated ligand placement.

Contact: Jane Bearinger (925) 423-0321 (bearinger1@llnl.gov)

Microdosing paper published

Ken Turteltaub and Graham Bench, together with collaborators at Oregon State University, published a paper in the December 2009 issue of ***Cancer Prevention Research*** titled "Effects of chlorophyll and chlorophyllin on low-dose aflatoxin B1 pharmacokinetics in human volunteers." The study used atomic accelerator mass spectrometry to determine aflatoxin pharmacokinetic parameters previously unavailable for humans, and suggests that chlorophyll and chlorophyllin co-consumption may limit the bioavailability of ingested aflatoxin in humans, as had been found in animal models. An accompanying "Perspective" article in the journal comments that the study has "validated the approach of using microdoses in prevention-related study of protection against an environmental carcinogen."

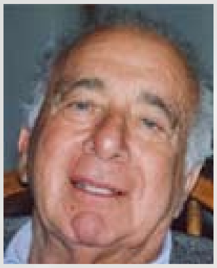
Contacts: Ken Turteltaub (925) 423-8152 (turteltaub2@llnl.gov) and Graham Bench (925) 423-5155 (bench1@llnl.gov)

People in the News

Valuing scientific excellence, leadership, and visibility

People in the News

Computational pioneer Alder receives National Medal of Science



Retired lab physicist and computational pioneer **Berni Alder** received the National Medal of Science. President Obama on September 17, 2009 named nine eminent researchers as recipients of the **National Medal of Science**, the highest honor bestowed by the United States government on scientists, engineers, and inventors. The awards were presented on October 7, 2009 at a White House ceremony. Alder is widely regarded as the founder of molecular dynamics, a type of computer simulation used for studying the motions and interactions of atoms over time. His expertise includes changing kinetic molecular theory by showing that simulations can significantly affect a scientific field. In 1980, Alder was one of the pioneers who used large-scale simulations to solve quantum mechanics problems. Alder said going into the field of molecular dynamics was "a relatively natural thing to do. The rest of the world didn't have access to the big computers." The National Medal of Science was created by statute in 1959 and is administered for the White House by the National Science Foundation. Awarded annually, the medal recognizes individuals who have made outstanding contributions to science and engineering. Nominees are selected by a committee of presidential appointees based on their advanced knowledge in, and contributions to, the biological, behavioral/social, and physical sciences, as well as chemistry, engineering, computing and mathematics. "These scientists, engineers and inventors are national icons, embodying the very best of American ingenuity and inspiring a new generation of thinkers and innovators," President Obama said. "Their extraordinary achievements strengthen our nation every day—not just intellectually and technologically, but economically, by helping create new industries and opportunities that others before them could never have imagined."

Alder did his undergraduate work at UC Berkeley and, in the late 1940s, studied for his Ph.D. at the California Institute of Technology, where he met computer designer Stan Frankel. Using CalTech's mechanical computers, Alder and Frankel developed a computer technique, now called the Monte Carlo method, for calculating results from random sampling. Alder continued developing his ideas at UC Berkeley and became a consultant to Lawrence Livermore when it opened in 1952 under Edward Teller's leadership. At the time, the connection to Livermore provided access to some of the only electronic computers in the nation. Alder joined LLNL full-time in 1955 and published his pioneering work on molecular dynamics in 1956. In 1963, Alder helped found the UC Davis Department of Applied Science, which offers undergraduate and graduate programs in physical sciences and engineering at UC Davis and at Livermore. Among numerous other honors, he also is a member of the National Academy of Sciences.

Today, molecular dynamics and Monte Carlo methods are widely used across a wide range of sciences, from fundamental physics to molecular biology. But at the time of Alder's work, those methods marked a radical change in how scientists thought about such problems. "It certainly exceeded any expectation I had to how far we could go and how big the computers would get," Alder said. "In the early days, we could do 100 particles in one hour on the Univac. Now, we can now do a trillion particles in an hour." Alder still works three afternoons a week at Livermore and two afternoons a week at UC Berkeley. "There are still problems I would like to solve. At Livermore there are some young people who are willing to work with me and help me solve some of these problems."

Reed receives Presidential Award for Excellence

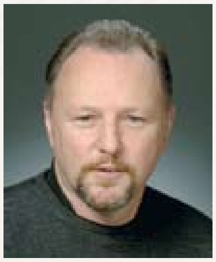
Kennedy Reed, a theoretical physicist at LLNL, was named by President Obama as a recipient of the prestigious **Presidential Award for Excellence in Science and Engineering Mentoring**. Reed works in research on atomic collisions in high-temperature plasmas. He has also been a leader in national efforts to increase opportunities for minority students and professionals in the sciences, and has been instrumental in the development of programs that have had national impact. Reed initiated and directed the Laboratory's Research Collaborations Program for Historically Black Colleges and Universities and Minority Institutions—an innovative program that links Laboratory scientists with professors and students in forefront research that benefits the Laboratory and universities. This program has strengthened the research and training capabilities at universities and has been very successful in encouraging student participants to pursue advanced degrees in science disciplines.

Reed also played a principal role in establishing the National Physical Science Consortium—a national coalition of corporations, national laboratories, and universities that provide graduate fellowships for women and minorities in the physical sciences. Reed has been widely honored for his work. He is a fellow of the American Physical Society. He was the 2003 recipient of the John Wheatley Award that cited his contributions to physics research and education in Africa. The California Section of the American Physical Society named an award in honor of Reed, and annually presents the Kennedy Reed Award for Best Theoretical Research by graduate students or postdoctoral researchers. Reed holds a bachelor of science degree at Monmouth College in Illinois, and a doctorate in physics at the University of Nebraska. The Presidential Award for Excellence in Science, Mathematics and Engineering Mentoring is awarded to individuals or organizations to recognize the crucial role that mentoring plays in the academic and personal development of students studying science or engineering and who belong to minorities that are underrepresented in those fields. The award was presented in a ceremony at the White House, and includes a grant of $10,000 to advance the recipient's mentoring efforts. "There is no higher calling than furthering the educational advancement of our nation's young people and encouraging and inspiring our next generation of leaders," President Obama said. "These awards represent a heartfelt salute of appreciation to a remarkable group of individuals who have devoted their lives and careers to helping others and in doing so have helped us all."

Goldstein named AAAS fellow

William Goldstein, associate director of PLS, was awarded the distinction of **American Association for the Advancement of Science (AAAS) fellow.** Election as a fellow is an honor bestowed upon AAAS members by their peers. In 2009, a total of 531 members were awarded this honor for their scientifically or socially distinguished efforts to advance science or its applications. New fellows were presented with an official certificate and a gold and blue (representing science and engineering, respectively) pin on February 20, 2010, at the AAAS Fellows Forum during the 2010 AAAS Annual Meeting in San Diego. This year's AAAS fellows were also announced in the "AAAS News & Notes" section of the December 18, 2009 edition of *Science*. As part of the physics section, Goldstein was elected for distinguished contributions to plasma modeling and diagnostics and for leadership in support of the Department of Energy national security programs. "This is a great honor that I owe largely to the Lab for the opportunity to contribute scientifically while addressing important national problems," Goldstein said. "I hope the fellowship will help me advocate for the critical role of science in international security." Early in his career, Goldstein co-authored and was among the first to apply a set of atomic modeling codes that have been used to significantly advance understanding of high-energy-density plasma properties through spectral modeling. The codes, developed at Hebrew University and LLNL, qualitatively improved modeling of atomic processes in plasmas, and have had impact in high-energy-density applications including x-ray lasers, high-energy astrophysics and fusion energy research. Goldstein went on to help develop the first spectroscopic diagnostics for astrophysical photoionized plasmas, designed some of the earliest laboratory astrophysics experiments using high-power lasers, and pioneered the use of detailed atomic models for predicting energy balance in Tokamaks. More recently, Goldstein has been a leader in the establishment and management of the Department of Energy's Stockpile Stewardship Program. Based on his experience using lasers in weapons physics research, he laid out the first systematic program of high-energy-density science for the National Ignition Facility. In his current position as the associate director for PLS, Goldstein leads the organization's approximately 600 scientists engaged in condensed matter and materials science, chemical science, atmospheric and earth systems science, high-energy-density physics, plasma physics, nuclear science, high-energy physics, radiation detection, optical science, biological science, and fusion research.

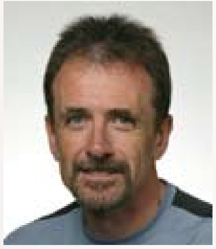
Researcher named AGU fellow



Rick Ryerson (AEED), leader of the Basic Energy Sciences–Geosciences Program, has been named a **Fellow** of the **American Geophysical Union** (AGU), a worldwide scientific community that advances the understanding of Earth and space for the benefit of humanity. Ryerson's citation reads: "for contributions to our understanding of transport processes in minerals, magmas, and crustal rocks at all scales." Ryerson's current work includes mineral–fluid equilibrium and diffusion kinetics in the Earth's interior, focusing on geochemical applications of high spatial resolution secondary-ion mass spectrometry. "I've been very fortunate to have had a long association with Livermore's branch of the Institute of Geophysics and Planetary Physics [IGPP]," says Reyerson. "The IGPP and the Laboratory Directed Research and Development Program allowed me to support an energetic group of postdocs and students, foster collaborations with various University of California campuses, and help to provide access to unique Lab facilities such as the Center for Accelerator Mass Spectrometry." AGU awards fellowships to scientists who have attained acknowledged eminence in one or more branches of geophysics. It elects no more than one-tenth of a percent of its membership as fellows.

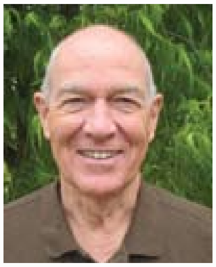
Researchers named APS fellows

Five LLNL researchers joined the ranks of the more than 200 American Physical Society (APS) fellows in 2009. APS fellowships are a distinct honor given after extensive review. Election to APS fellowship is limited to no more than one half of one percent of the APS membership for a given year. Receiving a fellowship reflects the honor and approbation of one's professional peers. This year, more than 200 members were elected APS fellows. The 2009 LLNL recipients were all current or former PLS employees:



David K. Bradley, a physicist in the Shock Physics Group. Bradley, who has been at the Lab for 11 years, was honored for "the development and use of high speed optical and X-ray instrumentation to discover new phenomena in high-energy-density plasmas."

Laurence Fried, a group leader in the Chemical Sciences Division, has been at LLNL 17 years and was recognized for "outstanding contributions to the physics and chemistry of shocked materials, the high-pressure, high-temperature equations of state of solids and liquids, and the prediction of energetic material reactivity, most notably the existence of sub-picosecond chemistry in high temperature dense fluids."



Arthur Molvik, a Lab retiree since July 2007 who worked in the Fusion Energy Program, was honored for "outstanding contributions to diverse areas of plasma physics and technology, including MHD stability limits in mirrors, and the physics of gas and electron accumulation in the ion accelerators."

Christine Orme, a staff scientist in the Biosciences and Biotechnology Division, was honored for her "outstanding contributions in understanding the fundamental physics of crystallization and materials assembly with application to biomineralizaion, biomimetic synthesis, and shape control of nanostructures."

Scott Wilks, a research scientist in the Physics Division, was honored for "pioneering contributions to the understanding of intense and ultra-intense laser plasma interactions and their applications to high-energy density science, including fast ignition, ion acceleration, and positron generation."

Papers share AAAS Newcomb Cleveland Award

A Laboratory researcher's paper published in November 2008 is a cowinner of this year's American Association for the Advancement of Science **Newcomb Cleveland Prize**. The paper is one of two outstanding papers published in *Science* from June 1, 2008, through May 31, 2009. **Bruce Macintosh**, of the Physics Division, is one of the lead authors for the paper entitled "Direct imaging of multiple planets orbiting the Star HR 8799," which appeared in the November 28, 2008, edition of *Science*. Christian Marois, a former Livermore postdoctoral researcher now at the National Research Council's Herzberg Institute of Astrophysics in Canada, is the other lead author. The Macintosh–Marois paper details how astronomers for the first time took snapshots of a multiplanet solar system, much like ours, orbiting another star. The new solar system orbits a dusty young star named HR 8799, which is 140 light years away and about 1.5 times the size of our Sun. Three planets, roughly 7 to 10 times the mass of Jupiter, orbit the star. Another paper—"Images of an Exosolar Planet 25 Light-Years from Earth," which appeared in the same issue of *Science*—shares the award. That paper includes Physics Division author Mike Fitzgerald, with Paul Kalas of the University of California at Berkeley as the lead author.

Gamma-ray detector wins R&D 100 Award

Physicist **Morgan Burks** was part of a team of scientists and engineers that developed GeMini—a portable gamma-ray spectrometer based on germanium technology—which was one of eight LLNL technologies honored by *R&D Magazine* with an **R&D 100 Award** for 2008. The GeMini instrument is so small that it fits in the palm of a hand, and this spectrometer is outfitted with an innovative low-powered, miniature cooling mechanism. GeMini was launched on NASA's Mercury MESSENGER spacecraft and is now taking the first-ever gamma-ray data of the planet Mercury. GeMini also can be used to help prevent smuggling of nuclear materials and can help in the implementation of international safeguards of nuclear fuel cycle facilities. This work was supported by the Defense Threat Reduction Agency and the NNSA Office of Dismantlement and Transparency in support of the Next Generation Safeguards Initiative. The R&D 100 Awards, often dubbed the "Oscars of invention," recognize the top 100 industrial innovations worldwide—advanced technologies with commercial potential. The

Development team for GeMini (from left): Dennis Carr, Morgan Burks, Marianne Ammendolia, and Livermore retiree Del Eckels.

winning of an R&D 100 Award provides a mark of excellence known to industry, government and academia and represents one of the most innovative ideas of the year.

Awards for technology transfers

Of the three awards for **Excellence In Technology Transfer** from the Federal Laboratory Consortium (FLC) won by LLNL—the most won this year by any laboratory among the more than 250 federal government laboratories and research centers in the consortium—PLS researchers were involved in two. Started in 1974, the Federal Laboratory Consortium assists the U.S. public and private sectors in utilizing technologies developed by federal government research laboratories.

Removing silica from geothermal waters. A team of scientists developed a technology that filters out silica from geothermal waters, allowing geothermal electrical plants to work more efficiently and to market a by-product, silica. While the United States leads the world in geothermal electrical production, one problem faced in geothermal turbine facilities is that silica clogs the pipes, filters, and heat exchangers. Still, the silica can be recovered and sold to manufacturers of products such as paint, paper, toothpaste, tires, dehumidifiers, and even solar photovoltaic cells. Although energy companies are normally focused on power generation and regard the geothermal brines as a troublesome waste product, the LLNL technology can not only solve the silica clogging problem, it can help mine out silica and other valuable minerals such as lithium (used in electric car batteries), manganese, zinc, and tungsten. The Livermore scientists conducted a field demonstration at Mammoth Pacific LP's geothermal power facility near Mammoth Lakes to show how the combination of their silica extraction process and reverse osmosis could improve plant efficiency and extract valuable metals. Pleasanton-based

Simbol Mining is bringing the technology to the marketplace. In March of 2008, Simbol's president presented the firm's business plan to the San Francisco Clean Tech Conference, and it was voted to be the most promising technology presented at the conference. Those receiving awards for the silica mining effort are former LLNL researchers **Bill Bourcier** (of AEED) (left) and **Carol Bruton** (of AEED) (shown in photo above; now at Simbol); LLNL business development executive Leah Rogers; LLNL patent attorney Eddie Scott; Cindy Atkins-Duffin of Global Security; and Simbol President Luka Erceg.

Maritime test bed aids security. A maritime test bed, set up in conjunction with the Monterey, CA-based Naval Postgraduate School, allows maritime security exercises to be conducted based on real-life scenarios. This award was shared by the Laboratory, the Naval Postgraduate School, Goleta, CA–based Textron Systems, Mill Valley, CA–based SecureBox Corporation, and an Oak Ridge National Laboratory researcher. "We have used this test bed to familiarize our licensees with the needs of first responders and other governmental users of technologies," said Annemarie Meike, a business development executive in LLNL's Industrial Partnerships Office. The team has focused on the need for improved internal cargo security and radiation detection, emphasizing tests with real end-users to identify, develop, field test and mature a series of technologies targeted toward maritime applications with a low false alarm rate. One of the technologies studied under the test bed and now headed into the marketplace is a cargo intrusion detector, designed to improve the security of cargo containers during shipping. The detector is a low-cost, reliable, reusable system that detects intrusions through any of the container's six walls. Another maritime security technology that has become commercially available is Textron Systems' Adaptable Radiation Area Monitor (ARAM), a radiation detector that can identify nuclear materials. The firm's ARAM Radboat became available in 2007. (The photograph shows a New Jersey State Police patrol boat, outfitted with ARAM technology, participating in a maritime test bed exercise in 2008 in New Jersey harbor.) Those who received the award are LLNL employees Bill Dunlop, Arden Dougan, **Dave Trombino** (of CSD), Kique Romero, and Peter Haugen; retired LLNL employee Norm Madden; LLNL business development executive Annemarie Meike; Frank Swanson and Brian Adlawan of Textron Systems; former CSD

scientist **Dan Archer** of Oak Ridge National Laboratory; Douglas Franco and Dirk Langeveld of SecureBox; and Alex Bordetsky of the Naval Postgraduate School.

Tech transfers recognized regionally

Laboratory scientists and engineers captured two outstanding **partnership awards** and two outstanding **technology development honors** in the **Federal Laboratory Consortium's Far West Region** competition.

One of the Laboratory's two **outstanding partnership awards** went to a team led by **Morgan Burks** (Physics Division) that developed GeMini, a portable gamma-ray spectrometer based on germanium technology. Small enough to fit in the palm of a hand, this spectrometer is equipped with an innovative low-powered, miniature cooling mechanism. The second outstanding partnership award was received for the large area imager, a radiation detection technology that

assists in locating illegal nuclear materials. Livermore researchers, including **Simon Labov** (Physics Division), worked with Oak Ridge National Laboratory and Science Applications International Corporation through funding from the U.S. Department of Homeland Security to deliver a commercial prototype. Among the large area imager's superior features are unprecedented sensitivity to weak sources, a minimum 5-fold increase in searching range, and a 25-fold speed-up in search time.

The Advanced Vision Systems for Minimally-Invasive Surgeries Project received one of

the Laboratory's two Far West Region awards for **outstanding technology development**. This effort, by Livermore **Stavros Demos** (CMMD), whose project is part of the Laboratory's collaboration with the University of California at Davis Cancer Center, provides surgeons with a real-time view of the critical tissue structure during gallbladder surgery. The Laboratory's other award for outstanding technology development was garnered by researchers who have been developing carbon nanotubes for water desalination and filtration. During their research, the team found the carbon nanotube membranes demonstrated permeability that is significantly higher than conventional membranes, despite having smaller pore sizes. The new technology offers several potential advantages over existing water filtration technology. Members of the carbon nanotube team include **Francesco Fornasiero** (BBTD) and former PLS employees **Olgica Bakajin, Aleksandr Noy, Jason Holt**, and **Hyung Gyu Park.**

Postdoc receives award from Colorado School of Mines

CSD postdoc **Ruth Tinnacher** was chosen for the **Environmental Science and Engineering Outstanding Graduate Student Award** from the Colorado School of Mines. This award recognizes graduating M.S. and Ph.D. students "who have demonstrated a significant impact through outstanding academic performance, leadership and service, and other meritorious contributions." Ruth was one of two awardees selected from a pool of 43 eligible students who graduated in either December 2008 or May 2009.

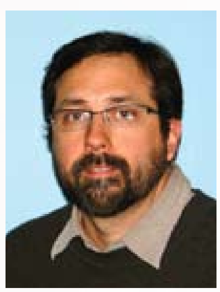
Two scientists garner DOE Early Career Awards

Grigory Bronevetsky, of Computation, and **Vsevolod Soukhanovskii**, of PLS, have both won a **DOE Early Career Research Program Award**. The two are among 69 scientists nationwide chosen to receive 5-year research grants funded under the American Recovery and Reinvestment Act. The award program is designed to bolster the nation's scientific workforce by providing support to exceptional researchers during the crucial early career years, when many scientists do their most formative work. Bronevetsky will focus his research on reliable high-performance peta- and exascale computing, and Soukhanovskii will conduct research in the Advanced High Heat Flux Diverter Program of the National Spherical Torus Experiment. Under the program, researchers based at DOE national laboratories receive grants of at least $500,000 per year to cover their salary and research expenses. To be eligible for an award, a researcher must be a full-time employee at a DOE national laboratory and have received a Ph.D. within the past 10 years. Awardees were selected from a pool of 1,750 applicants, who were selected by a committee of outside scientific experts.

Nuclear engineer recognized at DNDO awards

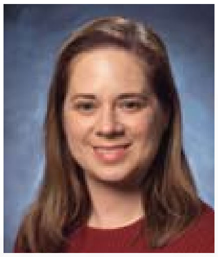
At a recent ceremony, the Domestic Nuclear Detection Office (DNDO) gave a **Director's Award** to **Frank Wong**, of PLS, and two colleagues, one from DNDO and one from the FBI. The award cited the team's contributions to the Office of the Director of National Intelligence (ODNI) Summer Hard Problem Program (SHARP) in the area of nuclear forensics and attribution. The team's results were briefed at very high levels, including the President's Special Assistant for Nuclear Defense and the Deputy Director for National Intelligence. Frank, the team's leader, was given exceptionally high praise from Bill Daitch, the DNDO assistant director, and Margaret Dillard, ODNI program manager. According to Dillard, Frank's project "is to date, the most robust and professional SHARP ever planned and executed." The picture shows, from left, DNDO Acting Deputy Director Bill Hagan; co-recipient Kristen Beahm, of DNDO; Frank; and Chuck Galloway, acting director of DNDO.

Seismologist heads to French Alps on Fulbright



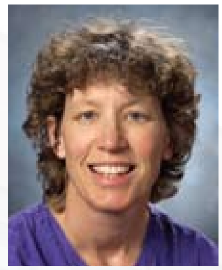
Artie Rodgers, head of PLS's Seismology Group, in the AEED, **received a Fulbright Scholarship** and headed to Grenoble, France, to study the relationship between topography and seismology with computer modeling. At Laboratoire de Géophysique Interne et Tectonophysique (LGIT), Université Joseph Fourier, Artie is using computational models of earthquakes and explosions to determine how free-surface topography impacts ground motion.

Chemist appointed to ACS Women Chemists Committee



Dawn Shaughnessy, a nuclear chemist in PLS, was recently named an **associate member of the American Chemical Society's Women Chemists Committee.** This is a joint committee of the Council and Board of Directors of the American Chemical Society. Dawn is also an alternate councilor of the society's Nuclear Chemistry and Technology Division.

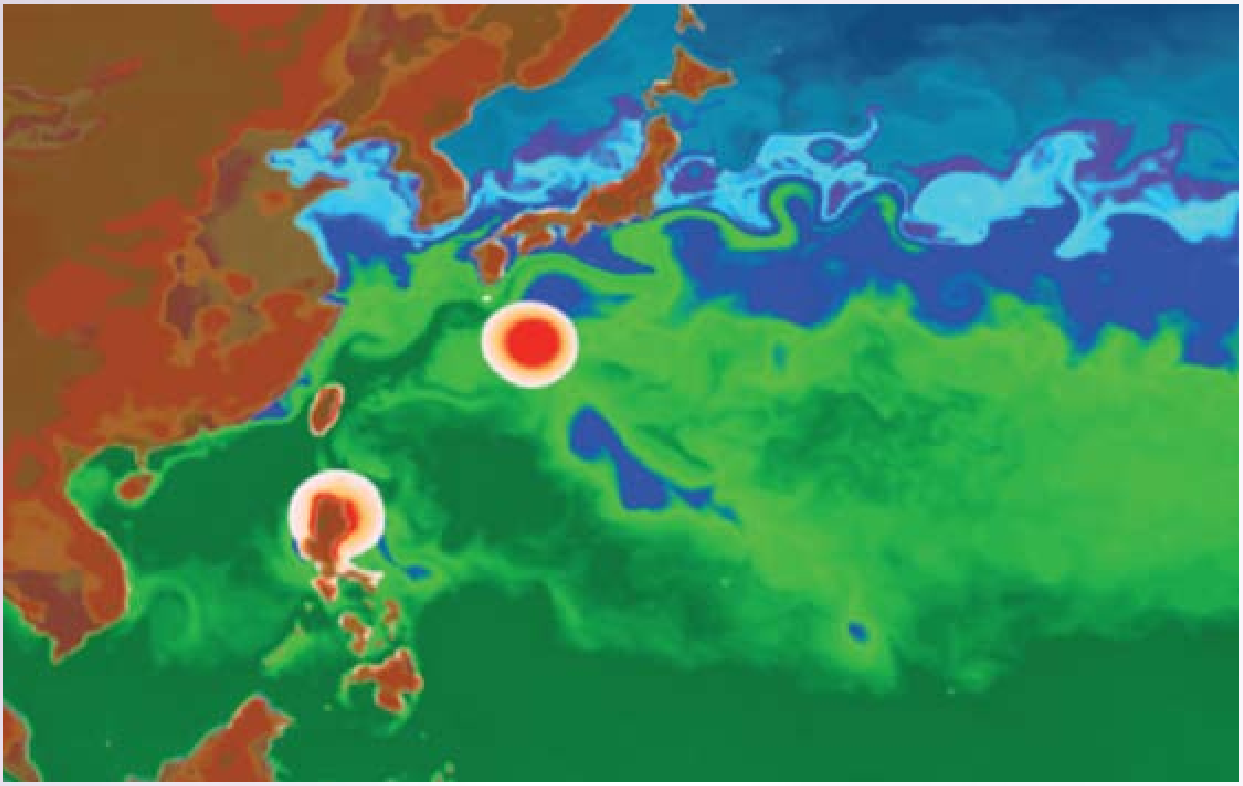
Plutonium poster wins award at international meeting



Migration '09 was the latest of an international meeting held every 2 years to showcase advances in understanding the chemistry and migration behavior of actinides and fission products in the geosphere. At the meeting, held in September at Washington State University, a poster by **Brian Powell** (a former LLNL postdoc currently at Clemson University) and PLS's **Zurong Dai, Mavrik Zavarin**, and **Annie Kersting**, titled "Plutonium colloid formation and structural association with minerals," **won one of three best poster awards** out of a total of over 200 posters that were presented at the meeting. The poster described research—funded by the postdoc program—on using transmission electron microscopy to interrogate the structure of plutonium sorbed onto colloids.

Researchers receive best poster award at conference

George Overturf, of CSD, and Constantine Hrousis and Michael Gresshoff, of the Engineering Directorate, shared a **best poster award** at the Institute for Chemical Technology (ICT) Energetic Materials Conference, held in July in Karlsruhe, Germany. The poster—"Probabilistic shock initiation thresholds and QMU applications"—received one of four awards presented at the conference. In the photo, Overturf (left) and Hrousis (middle) are receiving the award from Norbert Eisenreich (right) of ICT Fraunhofer.



Climate modeling effort wins major award

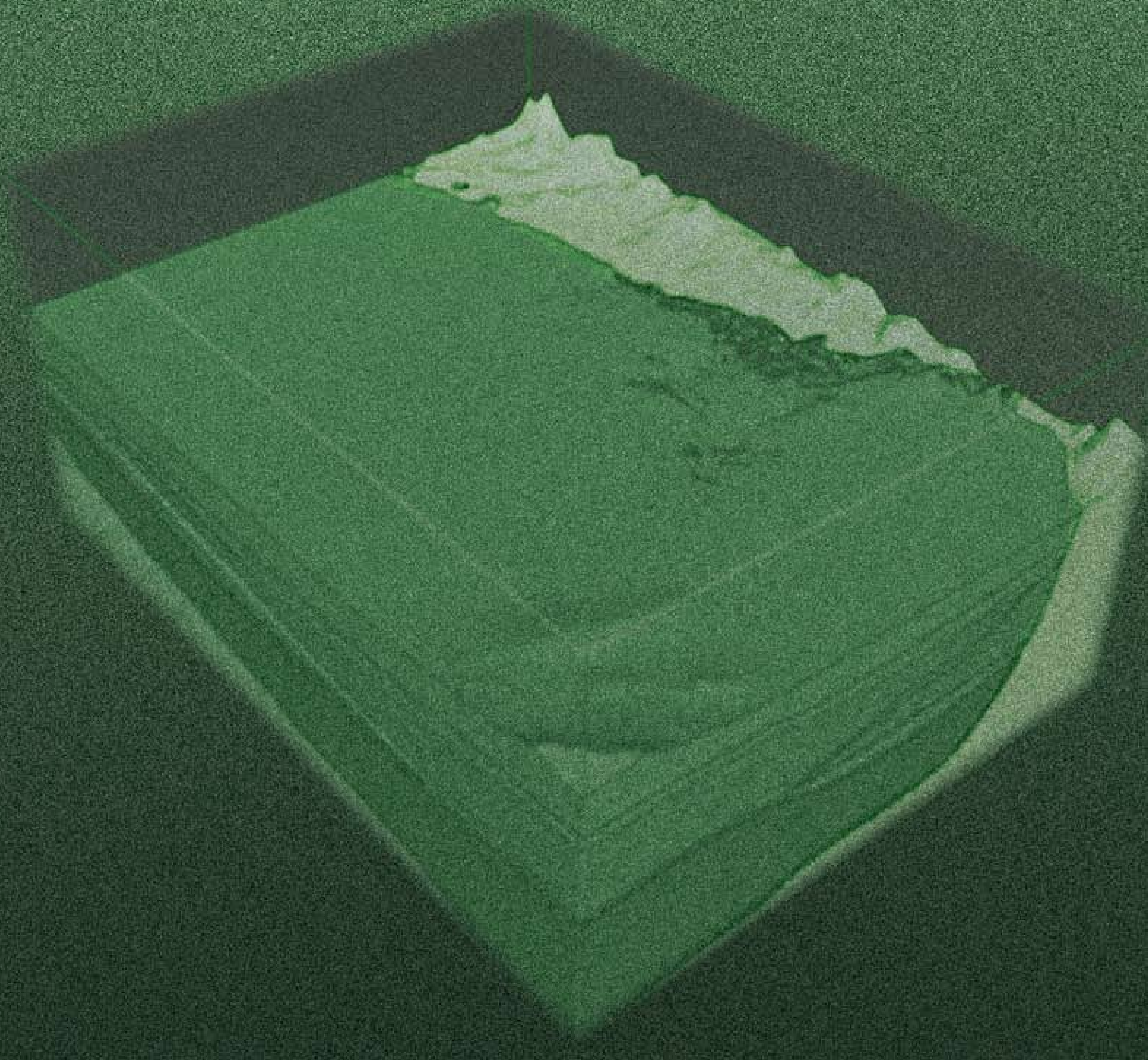
The Laboratory's Program for Climate Model Diagnostics and Intercomparison (PCMDI) was recognized by the **American Meteorological Society** (AMS) with a **special group award** for "leadership in implementing, maintaining and facilitating access to the Climate Research Program CMIP3 multi-model dataset archive, which led to a new era in climate system analysis and understanding." The award cites Dave Bader (formerly at LLNL), **Karl Taylor** and **Curt Covey** of AEED, and Jennifer Aquilino, Robert Drach, and Dean Williams of the Computation Directorate. The award was given at a January 20, 2010 AMS meeting. AMS President Tom Karl stated in his congratulatory email: "You have really changed the way we do business in climate science." The photo shows a PCMDI simulation of a tropical storm.

Publication ranks among top twelve accessed articles

A paper by chemist **Clark Souers** and his colleagues—"Air gaps, size effect, and corner-turning in ambient LX-17"—was published on January 8, 2009, in *Propellants, Explosives, Pyrotechnics* and was one of the **twelve most-accessed articles** at the entire Wiley InterScience website in March of that year.

Announcements in the News

Strengthening science and technology for national needs



Announcements in the News

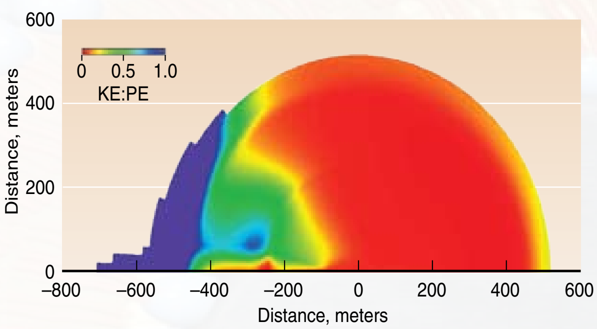
Carbon nanotube technology licensed for desalination

Lawrence Livermore exclusively licensed to Hayward, CA–based Porifera Incorporated a carbon nanotube technology that can be used to desalinate water and can be applied to other liquid-based separations. Carbon nanotubes—special molecules made of carbon atoms in a unique arrangement—allow liquids and gases to rapidly flow through, while the tiny pore size can block larger molecules, offering a cheaper way to remove salt from water. "The technology is very exciting," said Olgica Bakajin, a former LLNL employee who serves as chief technology officer of Porifera. "It's at the right place to take it to the marketplace." Porifera is developing membranes with vastly superior permeability, durability, and selectivity for water purification and other applications in the clean tech sector such as carbon sequestration. Bakajin and Francesco Fornasiero's (BBTD) research originally focused on using carbon nanotubes as a less expensive solution to desalination. Recently, the team made up of Bakajin and Francesco Fornasiero and Porifera scientists Sangil Kim and Jennifer Klare, thought about different applications for the nanotube membranes. "Carbon sequestration has always been at the back of our minds, as unique properties of carbon nanotube membranes provide critical advantages for potential use in carbon sequestration applications," Bakajin said. Bakajin agreed the membranes would separate CO_2 from nitrogen in power plant emissions. The membranes would transfer the two gases at a different rate so that the CO_2 could be separated and sequestered. Sequestering CO_2 is a key strategy to help curb global warming. "We've known about the possibilities for this for quite some time," she said. "The reason it makes sense to do it is because of the unique nanofluidic properties of carbon nanotube pores. We believe that our approach will work and we're looking forward to working with the Lab on this."

Contacts: Francesco Fornasiero (925) 422-0089 (fornasiero1@llnl.gov)

Analyzing the feasibility of using nuclear explosives to divert asteroids on a collision course with Earth

Scientists who study our solar system know that the seemingly fantastical idea of an asteroid impacting Earth and causing mass devastation is not just fodder for entertainment purposes; it is a real concern. To prevent such a catastrophic event, scientists across the nation, including Physics Division astrophysicist David Dearborn, are analyzing techniques to disrupt or divert asteroids on a collision course with Earth.



Simulation results show the effects of detonating a 1-kiloton nuclear explosive 150 meters above the surface of a 1-kilometer-diameter object. Colors indicate the ratio of kinetic energy (KE) to potential energy (PE) produced by the impact. The explosion obliterates the ejected debris (purple). In the bound areas (light blue to red), the object receives a "push," which changes its speed by a few centimeters per second.

As telescopes and other astronomical survey tools have become more precise, they have revealed that the number of asteroids within Earth's orbit is significantly greater than previously predicted. In addition, evidence of past impacts indicates that the collisions may have caused widespread devastation. In 1998, the National Aeronautics and Space Administration (NASA) started the Spaceguard Near-Earth Object Survey to acquire data on objects that orbit close to the Sun. The current NASA program has focused on finding 90% of the near Earth objects (NEOs) of a size greater than a kilometer. (NEOs are objects whose orbits approach the Earth closer than about half the distance to Mars.) So far the program has found more than 500,000 asteroids, of which 6,758 are classified as NEOs and 1,086 are potentially hazardous objects, with orbits that pass closer to Earth than about 20 times the distance to the Moon.

"An object of this size would have approximately 1 billion tons of mass," says Dearborn. "If it traveled at 30 kilometers per second, it would have explosive power equivalent to 100 billion tons of TNT." Dearborn serves on a research panel, spearheaded by the National Academy of Sciences, tasked with evaluating methods to divert potentially hazardous objects—those that could hit Earth in the next 100 years. The panel is considering several diversion technologies, but for Dearborn, nuclear explosives provide the best solution for dealing with catastrophic asteroids.

Such an event can be avoided by nudging the asteroid off course or by fragmenting it. The action needed depends on the object's size and the time available before impact. According to Dearborn, nuclear explosives are the optimal method for diverting large asteroids or those that are too close to Earth—less than a decade away in time—to be deflected through other means. One benefit is that nuclear explosives are an established technology. "They are well tested and characterized," says Dearborn, "and the outputs and effects of explosions are well understood." In addition, nuclear explosives have a high energy-to-weight ratio, so they offer the lowest mass method for transporting energy to the asteroid.

To evaluate the effectiveness of different approaches, Dearborn and his colleagues used the Laboratory's multidimensional hydrodynamic codes to simulate three scenarios in which a nuclear explosive diverts an inhomogeneous, 1-kilometer-diameter structure. For each scenario, the team altered nuclear outputs, explosives energies, distances from the object, and the height or depth at which the explosion occurs. The simulated results indicate that in all three scenarios, the fragments created would be small and fast enough to avoid collisions with Earth. Future studies will vary the simulated object's shape, density, and porosity to determine how an asteroid's composition affects the outcome.

Although there is some uncertainty in determining exactly when and where an asteroid could impact the planet, Dearborn notes that no asteroid currently being monitored poses an immediate threat. "But that doesn't mean we shouldn't have a deflection plan in place," he says. And nuclear explosives may prove to be the best technology for the job.

Contact: David S. Dearborn (925) 422-7219 (dearborn2@llnl.gov)

GeMini in the news

A story on ABC-7 News on December 13 featured Morgan Burks (PLS) describing the GeMini radiation detector. The GeMini development team, led by Morgan, received a 2008 R&D 100 Award for this innovative technology.

Contact: Morgan Burks (925) 423-2798 (burks5@llnl.gov)

Geophysicist installs world's deepest electrical resistance tomography system

Charles Carrigan, of PLS, and his colleagues installed an electrical resistance tomography (ERT) array to depths of more than 10,000 feet to monitor CO_2 injection for the Southeast Regional Carbon Sequestration Partnership (SECARB) project in the Cranfield Field in southwest Mississippi. This new ERT system—the world's deepest—images the growth and movement of CO_2 plumes as they move from the subsurface injection point. The SECARB effort involves the greatest injection ever achieved in the US—1,158,858 metric tons as of September 30, 2009—and is only the fifth carbon sequestration project in the world to reach the million-ton mark. DOE issued a press release recognizing SECARB for furthering CO_2 capture and storage technology and for meeting G-8 goals for demonstrating this capability by 2010.

Contact: Charles Carrigan (925) 422-3941 (carrigan1@llnl.gov)

Multi-lab climate proposal funded

DOE has awarded funding to a joint LLNL–LANL–ORNL proposal titled "Ultrahigh-resolution global climate simulations to explore and quantify predictive skill for climate means, variability, and extremes." Ken Sperber, of PLS, is serving as project leader at LLNL, which is receiving $525,000 per year for up to 5 years. With this new funding, the Program for Climate Model Diagnosis and Intercomparison will develop new metrics and diagnostics to evaluate ultrahigh-resolution, coupled ocean–atmosphere preindustrial, present-day, and climate change simulations performed at ORNL. The simulations will be compared against those in which either or both of the component atmospheric and ocean models are run at lower resolution. These simulations will test the scale sensitivity of the models' physics and assess the impact of using different dynamical cores, with special attention given to the evaluation of hydrological processes.

Contact: Ken Sperber (925) 422-7720 (sperber1@llnl.gov)

Researcher receives funding to study aging of the human eye lens

Bruce Buchholz, of PLS, has been awarded funding from the National Eye Institute of the National Institutes of Health to quantitate protein turnover in the human adult eye lens using the carbon-14 bomb pulse, a method pioneered by Buchholz and his collaborators at Sweden's Karolinska Institute and previously applied to fat cell and neuron turnover. The project will involve isolating proteins from human lens samples and evaluating protein age by means of carbon-14 accelerator mass spectrometry to estimate the level of protein turnover.

Contact: (925) 422-1739 (buchholz2@llnl.gov)

Geothermal energy program revitalized with new funding

Twenty years ago, LLNL had a thriving geothermal program. But as funding dwindled, the program did as well. But thanks to a new flow of money from DOE's Geothermal Technologies Program Office, the LLNL research will soon flourish again. The new funding reflects recent trends such as high oil prices and increased emphasis on non-carbon-releasing sources of energy.

Postdoc Dennise Templeton is using the funding for her project to map microseismicity for geothermal reservoir management. The project is aimed at detecting and locating microearthquakes induced by EGS hydrofracturing and fluid reinjection operations within the reservoirs. "Accurate identification and mapping of the large numbers of microearthquakes caused by geothermal production can provide us with diagnostic information so we can determine the location, orientation and length of underground crack systems for reservoir development and management applications," Templeton said. In EGS, water is initially pumped into the ground at high pressures. Templeton said when this fluid is pumped underground, cracks form, which enhances the existing permeability of the rock. After the underground fracture network is developed, cold water can be reinjected at lower pressures, heated by the host rock, and extracted from a production well as extremely hot water. This hot water can then be converted into electricity in geothermal power plants. Using seismic tools, she and her team can locate where the cracks are initially forming and the possible locations of the reinjected fluids by tracking the microseismicity. In the next phase of her project she will take data generated at existing geothermal locations and conduct the seismicity analysis in real time.

Geochemist Susan Carroll is using the program funding to determine what effect geochemical reactions have on the use of carbon dioxide (CO_2) as an efficient heat exchanger for geothermal energy production. "We want to understand what impact CO_2 would have on geochemical reactions and how it would affect the field, whether it would enhance or clog fracture networks that bring heat to the surface," she said. Earlier research has shown that using supercritical CO_2 instead of water as a heat transfer fluid yields significantly greater heat extraction rates for geothermal energy. If this technology is implemented successfully, it could increase geothermal energy production and offset atmospheric emissions of greenhouse gases. But the impact of geochemical reactions between acidic waters in equilibrium with supercritical CO_2 and the reservoir rock have not been assessed. Carroll's project consists of three phases: assessing the geochemical impact of CO_2 on geothermal energy production by analyzing the geochemistry of existing geothermal fields with elevated natural CO_2; measuring realistic rock–water rates for geothermal systems using laboratory and field-based experiments; and developing reactive transport models using the field-based rates to simulate production scale impacts, if any. "If CO_2 is a better heat exchanger we'd be using a greenhouse gas to produce energy that is carbon free," Carroll said. DOE's budget for geothermal energy has fluctuated during the last decade going from about $22 million per year, down to $5 million in 2007 and then bounced up to $44 million in 2009. "People have realized that climate change is a real issue," said Jeff Roberts, who leads the Alternative Resource Cycles Program. "Everything has changed to work in favor of getting more renewable energy moving forward."

Contacts: Dennise Templeton (925) 422-2021 (templeton4@llnl.gov) and Susan Carroll (925) 423-5694 (carroll6@llnl.gov)

LLNL partners with Siemens to improve wind energy efficiency

Under a $2 million agreement signed with Siemens Energy, LLNL began providing numerical weather prediction models with resolution as fine as 1 kilometer to predict power generated by the wind so that wind farms can operate more efficiently while providing more power to hungry grids. Many U.S. wind parks are yielding up to 20 percent less energy than predicted because of uncertain forecasts. More accurate wind predictions will have a positive effect on wind farm operators and owners who can know hours or days ahead of time how wind conditions will affect power generation. "Knowing the certainty of the forecast can be useful in a day-ahead or futures market where now there are penalties for under-performance," said Julie Lundquist, a former PLS atmospheric scientist who was heading the project. LLNL has developed improved methods for simulating the turbulent properties of the lower atmosphere that should translate into a significant predictive advantage for wind energy applications. More accurate predictions also could reduce the investment risks in wind-powered projects, could improve the design of tall wind turbines to withstand the high turbulence environment higher in the atmosphere, and enable optimal bids on wind farm production. "Accurate and timely forecasts of power availability will enable turbine owners and operators to generate optimal bids on wind turbine production and in turn maximize both financial benefit and grid support," said Henrik Stiesdal, Siemens chief technology officer for wind power generation. "We look forward to this cooperative agreement that will help us provide a clean energy source for future generations."

The Department of Energy and Siemens recently signed a memorandum of understanding to work together on wind technology. "Through this agreement, wind manufacturers, DOE and our laboratories will enhance wind technology capability to be a competitive energy supply for America," said Steve Lindenberg, senior adviser for DOE's Renewable Energy Office. "Siemens' growing presence in this country and the partnership with a national laboratory like Lawrence Livermore helps provide a new opportunity to deploy a clean source of energy."

In addition to providing hourly and daily predictions, Livermore will explore impacts of global climate change on wind resources 20 years into the future. While the value of forecasting is hard to quantify, several studies have suggested that more accurate forecasting can render not only more clean energy but also enhanced profits for industry. A study performed by a member of the industry of the effect of 3,300 MW of wind generation in New York state quantified improved forecasting to be worth $125 million a year to that region. Based on a conservative application of this figure, Stiesdal estimates that wind farm owners may be able to increase revenue by as much as 10 percent, making wind power more profitable and ultimately reducing the cost of energy.

Contact: Jeff Roberts (925) 422-7108 (roberts17@llnl.gov)

Research agreement with Chevron

Chris Orme, of PLS, was principal investigator on a project that has led to a research agreement between LLNL and Chevron to develop the next generation of catalysts for the production of cleaner, more efficient fuels from crude oil. The research will focus on how catalytically active surfaces form and change on contact with feed molecules and, in particular, over time, how they are influenced by promoters and impurities. This work will utilize state-of-the art in situ methods to examine catalysts in realistic environments and will focus on specific catalysts that exhibit high reactivity and resistance to sulfur poisoning. Chevron would like to gain a better understanding of the promoter effects and impurity interactions at the atomic scale to improve catalyst efficiency, particularly effects of substitution of various metal atoms that influence catalyst selectivity and stability. LLNL's expertise in crystal growth and technical skills in the use of novel in situ surface techniques (such as atomic force microscopy) will enable Laboratory researchers to examine impurity interactions with catalytic surfaces at higher resolution than has been previously achieved.

Contact: Chris Orme (925) 423-9509 (orme1@llnl.gov)

Scientist chairs program committee for 2009 Sherwood Fusion Theory Conference

Tom Rognlien, of PLS, served as program committee chair for the 2009 Sherwood Fusion Theory Conference, which was colocated with the 2009 American Physical Society April Meeting in Denver, CO.

Contact: Tom Rognlien (925) 422-9830 (rognlien1@llnl.gov)

Scientist serves as co-organizer of "Evolution of Planets" symposium

Gilbert Collins, of PLS, and Professor Raymond Jeanloz, of UC Berkeley, co-organized a symposium titled "The Evolution of Planets" as part of the AAAS Annual Meeting in Chicago, February 12–16, 2009. The moderator was Tristan Guillot, of France's Centre National de la Recherche Scientifique. The symposium consisted of six 30-minute presentations: "The Search for Living Planets" (Alan P. Boss, Carnegie Institution for Science), "Formation of Terrestrial Planets" (Robin Canup, Southwest Research Institute), "Frontiers in the Interiors of Massive Planets" (David Stevenson, CalTech), "Exotic Behavior of Materials at Multimegabar Pressures" (Russell Hemley, Carnegie Institute), "Exploring Matter to Gbar Pressures" (Raymond Jeanloz, UC Berkeley), and "Recreating Planetary Core States with Quantum Molecular Dynamics" (Giulia Galli, UC Davis).

Contact: Gilbert Collins (925) 423-2204 (collins7@llnl.gov)

Scientists contribute chapter to Shock Wave S&T Reference Library

Larry Fried and Sorin Bastea, of PLS, were chosen to write a chapter for the book *Detonation*, part of the multivolume series "Shock Wave Science and Technology Reference Library." The chapter will be entitled "Chemical Equilibrium Theory of Detonation." *Detonation* will deal mainly with the fundamentals of gas and condensed-matter detonation, including equilibrium detonation, steady detonation structure, detonation instability, dynamic parameters of detonation, multiscaled cellular detonation, detonation shock dynamics, and the theory and practice of condensed matter detonation. The book will serve as a comprehensive handbook for scientists and engineers.

Contact: Larry Fried (925) 422-7796 (fried1@llnl.gov)

Researcher joins Fusion Energy Scientific Advisory Committee

Bruce Cohen, of PLS, was selected to become a member of the Fusion Energy Scientific Advisory Committee (FESAC), which provides independent advice to DOE's Office of Science on complex scientific and technological issues that arise in the planning, implementation, and management of the fusion energy sciences program. Committee members are drawn from universities, national laboratories, and private firms involved in fusion research. Members serve a 2-year term as Special Government Employees during their work on FESAC. Additional ex officio committee members include the chairs of APS Division of Plasma Physics and ANS Fusion Energy Division and a representative from the IEEE Executive Committee.

Contact: Bruce Cohen (925) 422-9823 (cohen1@llnl.gov)

Scientist chairs SPIE meeting

James Dunn, of PLS, was selected as a conference chair for SPIE's Conference on Soft X-Ray Lasers and Applications VIII, held in San Diego, CA, August 4–6. Dunn also chaired the previous meeting in 2007. The meeting is held every 2 years and is an ongoing series on plasma-based x-ray lasers and related research areas. Dunn served as conference co-chair with Professor Gregory J. Tallents of the University of York, United Kingdom. Ten oral and one poster sessions were held on topics including x-ray laser applications, recent free-electron laser research and higher order harmonic generation. Papers from the meeting were published in *Proceedings of SPIE* volume 7451, "Soft X-Ray Lasers and Applications VIII," which James and Gregory also edited.

Contact: Jim Dunn (925) 423-1557 (dunn6@llnl.gov)

History Channel cites LLNL Loch Ness science

Thomas Guilderson, of AEED, appeared in the History Channel documentary “MonsterQuest: Death of Loch Ness.” The segment, aired on February 4, 2009, included both footage of CAMS and Guilderson’s description of the carbon dating results of shells collected from Loch Ness—work performed approximately 5 years ago. Age data provides the best evidence to date that Loch Ness likely contained marine organisms during the era of glacial retreat at the end of the last ice age—supporting speculation that the “monster” may be descended from a large prehistoric ocean-dwelling species.

Contacts: Thomas Guilderson (925) 422-1753 (guilderson1@llnl.gov) and Thomas Brown (925) 423-8507 (brown92@llnl.gov)

Funding approved for Heavy Ion Fusion Facility in collaboration with LBNL and PPPL

The Heavy Ion Fusion Science Virtual National Laboratory, a collaboration of PLS’s Fusion Energy Program with LBNL and the Princeton Plasma Physics Laboratory (PPPL), received approval for construction of the second-phase Neutralized Drift Compression Experiment (NDCX-II) at LBNL, with completion anticipated by March 2012. The goal is to deliver 30–50 nC of ions at energies ranging from 1 to 3 MeV in about 500 ps into a sub-millimeter-radius spot on a variety of targets. Applications of this facility will include studies of the basic physics of the warm dense matter regime in foils heated uniformly (from front to back) by ions with energies near the Bragg deposition peak; exploration of ion-energy coupling into an ablating plasma using beams with ramped kinetic energy; investigation of the dynamics of space-charge-dominated ion beams; and research on beam focusing and pulse compression in a neutralizing plasma environment. Many of these studies will contribute directly toward the collaboration’s ultimate goal of achieving heavy-ion fusion: production of electric power via inertial-confinement fusion driven by heavy-ion beams.

Contact Alex Friedman (510) 486-5592 (friedman1@llnl.gov)

Team rates labs from 19 nations on chemical weapon sample analysis

Armando Alcaraz (CSD) and Hugh Gregg (AEED) had a central role in a February 12, 2009 meeting organized by the Organization for the Prohibition of Chemical Weapons (OPCW), held at The Hague. At the meeting, the two chemists reported the results of the Forensic Science Center’s evaluation of the reports resulting from the 24th OPCW Proficiency Test, which tests the proficiency of participating laboratories in analyzing chemical weapon-related samples. Twenty-three laboratories, representing 19 different countries, participated in the test. Only eleven of the labs correctly identified all six chemicals of interest. None of the OPCW-accredited laboratories lost accreditation as a result of scores from this test round.

Contacts: Hugh Gregg (925) 423-7501 (gregg2@llnl.gov) and Armando Alcaraz (925) 423-6889 (alcaraz1@llnl.gov)

Scientist becomes adjunct professor to expand LLNL–CSU Education Partnership

Don Correll, PLS Fusion Energy Program Leader, accepted an offer from the Physics Department at California State University (CSU) East Bay to become an adjunct professor. Don is helping to expand the collaboration between LLNL and the CSU system of 23 campuses. In addition, LLNL, through a collaborative partnership between the CSU, other national laboratories, and the NASA Ames Research Center, is expanding the Science Teacher and Researcher summer internship program for pre-service and early-career science teachers teaching or planning to teach in the 6th through 12th grades.

Contact: Don Correll (925) 422-6784 (correll1@llnl.gov)

Scientist honored in special session of ACS Nuclear Chemistry and Technology Division

The Nuclear Chemistry and Technology Division of the American Chemical Society held a special session honoring PLS scientist Ken Moody at its Spring 2009 Meeting in Salt Lake City, March 22–26, 2009. The 4-hour session—"Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Kenton J. Moody"—featured a 1-hour talk by Moody followed by six 30-minute talks. The session was chaired by PLS scientist Mark Stoyer in his role as chair of the Nuclear Chemistry and Technology Division. The theme of the overall conference was "Nanoscience: Challenges for the Future," which included topics from nanotechnology to analytical chemistry to medicinal R&D and covered research advances described in 7,275 published papers.

Contact: Ken Moody (925) 423-4585 (moody3@llnl.gov)

Scientist serves on DOE Basic Energy Sciences Review Committee

Geoffrey Campbell, of CMMD, was selected to join the Committee of Visitors of DOE's Office of Basic Energy Sciences (BES). The committee reviews management processes in the BES Materials Science and Engineering Division. This includes assessing processes for soliciting proposals, awarding contracts, and monitoring programs, as well as the breadth and depth of the portfolio and the national and international standing of portfolio elements. The committee's input will be used by the Office of Management and Budget to assess progress towards long-term goals and by the Office of Science for process improvement.

Contact: Geoffrey Campbell (925) 423-8276 (campbell7@llnl.gov)

Lawrence scholar named top student presenter at seismology conference

Dylan Rood, a Lawrence scholar in AEED, was selected as a top student presenter at the Seismological Society of America conference held April 8–10, 2009, in Monterey, CA. This honor—which is awarded to only 10 to 15 percent of all student presenters each year—will be announced in an upcoming issue of *Seismological Research Letters*. Dylan was selected for his oral presentation, titled "Dating offset alluvial fans along the San Andreas Fault in the Santa Cruz Mountains using LiDAR and Be-10 geochronology."

Contact: Dylan Rood (925) 422-7378 (rood5@llnl.gov)

Scientist appointed to decadal astronomy survey

Physics Division scientist Bruce Macintosh has been appointed to the Optical and Infrared Astronomy from the Ground Panel of the Astronomy and Astrophysics 2010 Decadal Survey. This is a full national review—the latest in a series of surveys that are produced every 10 years by the National Research Council of The National Academy of Sciences—setting out research priorities and strategy for the next 10 years of ground- and space-based astronomy.

Contact: Bruce Macintosh (925) 423-8129 (macintosh1@llnl.gov)

Scientist appointed to Astro-H science working group

PLS scientist Greg Brown has been selected as a member in the Astro-H Mission (formerly known as the New Exploration X-ray Telescope) Science Working Group, which was created by NASA and the Japan Aerospace Exploration Agency to provide scientific guidance to the Astro-H Project on the design, development, and operations phases of the mission. The working group includes individuals from both the instrument teams and the broader astrophysics community. Greg will focus mainly on calibration of the soft x-ray spectroscopy system.

Contact: Greg Brown (925) 422-6879 (brown86@llnl.gov)

Scientist joins IAU committee

Peter Beiersdorfer, of the Physics Division, was selected to become a member of the International Astronomical Union (IAU) Commission 14 Organizing Committee. This became effective after the IAU General Assembly in Rio de Janeiro in August 2009. The term of service is typically two consecutive 3-year periods. Beiersdorfer's name was included among the names of the committee and officers submitted to the IAU Executive Committee for final approval at the General Assembly. Commission 14 deals with atomic and molecular data for astronomy.

Contact: Peter Beiersdorfer (925) 423-3985 (beiersdorfer1@llnl.gov)

Breakthrough has possible anthrax research applications

In a development that could have a major impact on anthrax research, BBTD researchers discovered a new process for releasing cell DNA. The researchers—Feliza Bourguet, Matthew Coleman, Brian Souza, and Paul Jackson—discovered an endolysn-encoding gene in a pathogenic *Bacillus cereus* isolate. Endolysins, including a group known as muramidases, are a family of enzymes that, under normal circumstances, introduce nicks in the structure of bacterial cell walls. However, in high concentrations they lead to rapid cell lysis, with release of cellular content. The results are important to researchers at the Centers for Disease Control (CDC) on the antibiotic resistance of *B. anthracis* (the anthrax pathogen) as this research requires the rapid and complete lysis of bacterial cells to release DNA for assays. After testing LLNL's muramidase, the CDC indicated its desire to establish an agreement with LLNL to use this protein in assays that will be distributed to all laboratories in the Laboratory Response Network. Successful early testing of this lytic protein at CDC was followed by large-scale production of the protein at the CDC core production facility. The protein has been shown to be fully functional after lyophilization (freeze drying) and promises to be highly stable. CDC investigators have recently requested permission to share the protein with scientists at the United States Army Medical Research Institute for Infectious Diseases, where investigators plan to use it in similar assays requiring complete cell lysis.

Contact: Feliza Bourguet (925) 424-5666 (bourguet1@llnl.gov)

Scientists involved in four Energy Frontier Research Centers

PLS scientists in 2009 worked as co-investigators with four Energy Frontier Research Centers (EFRCs): the Center for Nanoscale Control of Geologic CO_2 at LBNL, the Center for Energy Frontier Research in Extreme Environments at the Carnegie Institution of Washington, the Center for Extreme Environment-Tolerant Materials via Atomic Scale Design of Interfaces at LANL, and the Energy Frontier Center for Defect Physics in Structural Materials at ORNL. In a major effort to accelerate the scientific breakthroughs needed to build a new 21st century energy economy, a total of 46 EFRCs have been established at universities, national laboratories, nonprofit organizations, and private firms across the nation. DOE's Office of Science plans to invest over $700 million in the EFRCs over the next 5 years.

Contact: Henry Shaw (925) 423-4645 (shaw4@llnl.gov)

Distant galaxy imaged

As part of an effort to more accurately measure the expansion of the universe by looking at Cepheid variable stars in a distant galaxy, Kem Cook, formerly of PLS Physics Division, and colleagues helped create an exceptionally deep view of a strange galaxy. Using images from NASA's Hubble Space Telescope, they have generated an unprecedentedly clear view of the unusual spiral galaxy NGC 4921. Cook and his colleagues have been studying the variable stars in this galaxy since 2007. His team was using Hubble to search for Cepheid variable stars in NGC 4921 that could be used to measure the expansion rate of the universe. The final image created in 2009 was from 50 separate exposures taken from late 2007 through early 2008 using a yellow visible light filter and another 30 exposures through a near-infrared filter using Hubble's Advanced Camera for Surveys. The total exposure times were approximately 17 hours and 10 hours, respectively. The galaxy is part of the Coma Galaxy Cluster, which is about 320 million light-years from Earth. Cook's team—which consisted of members from LLNL, the University of California at Davis, Texas A&M University, McMaster University, and the Herzberg Institute of Astrophysics—made initial images of the same galaxy during earlier studies. The image is a result of work by the Space Telescope Science Institute, the science operations center for the Hubble Space Telescope, the European Southern Observatory, and the European Space Agency.

Conact: Kem Cook (925) 423-4634 (cook12@llnl.gov)

Scientist wins $2 million grant to develop electron microscope for biology

PLS scientist Nigel Browning and his UC Davis colleagues received a $2 million grant from the National Institutes of Health to develop the world's first electron microscope capable of filming live biological processes. The team's plan is to extend the capabilities of a dynamic transmission electron microscope (DTEM) to capture 10 to 100 images per millionth of a second while also capturing details as small as 10 nm (about four times the diameter of a DNA molecule). Currently, there are only three DTEMs in use worldwide, none of which are designed for observing living systems. Browning and his team will be building a "Bio-DTEM" that will incorporate three new elements: a custom-built system to hold an ultrathin layer of fluid containing the biological sample to be imaged, a short-exposure-time imaging mode to avoid the blurring problem created when molecules move through their fluid medium, and a new generation of scientific instrumentation to deliver optimum image contrast for biological samples and to correct image distortions generated by lenses. In July 2009, Browning added an appointment in the Department of Molecular and Cellular Biology to his academic positions at UC Davis.

Contact: Nigel Browning (925) 424-5563 (browning20@llnl.gov)

Researchers receive NASA funding to upgrade Focused Ion Beam

As part of a 3-year cosmochemistry grant she was awarded, PLS scientist Hope Ishii received a $230,000 grant from NASA to upgrade the capabilities of LLNL's Focused Ion Beam (FIB) instrument. Hope and her collaborators will use the new capabilities to rapidly prepare better quality, highly localized transmission electron microscopy samples of meteorite specimens to improve understanding of the materials processing that occurred in the early solar nebula and on meteorite parent bodies. This upgrade, combined with previous state-of-the-art modifications, will make the LLNL FIB one of the most powerful instruments of its kind.

Contact: Hope Ishii (925) 422-7927 (ishii2@llnl.gov)

Scientist invited to organize symposium at crystal growth conference

PLS scientist S. Roger Qiu was invited to organize a symposium at the 17th American Conference on Crystal Growth and Epitaxy, which was held August 9–14, 2009, at Lake Geneva, WI. The symposium provided a forum for the presentation and discussion of recent research and development activities in all aspects of biocrystallization and bioinspired synthesis of crystalline materials for technological and medical applications. Sessions integrated fundamental, experimental, and industrial growth processes, as well as characterization and applications.

Contact: S. Roger Qiu (925) 422-1636 (qiu2@llnl.gov)

Scientist elected to ANS committee

PLS scientist Lucile Dauffy was recently elected to the Executive Committee of the Fusion Energy Division of the American Nuclear Society. The division "promotes the development and timely introduction of fusion energy as a sustainable energy source with favorable economic, environmental, and safety attributes."

Contact: Lucile Dauffy (925) 422-6311 (dauffy1@llnl.gov)

Geophysicists participate in Test Ban Treaty activities

In October, William Walter (AEED), as a member of the Seismology Subcommittee for the National Academy of Sciences panel reviewing issues related to the Comprehensive Nuclear Test Ban Treaty (CTBT), met with Air Force Technical Applications Center officials in Florida and with DOE sponsors in Washington, D.C. In November Walter traveled to Vienna with panel members to meet with the CTBT Organization to discuss topics related to the international verification system being established as part of the CTBT.

Contact: William Walter (925) 423-8777 (walter5@llnl.gov)

Researcher featured in National Geographic documentary

Brooke Buddemeier, of CSD, was one of two Laboratory researchers featured in a one-hour documentary aired in November 2009 on the National Geographic Channel. The program, called "Dirty Bomb Attack," shows what would happen if a U.S. city were the target of a hypothetical radiological attack. The program starts with a dramatization of a car bomb detonating on a busy street and moves to the question of what happens next.

Contact: Brooke Buddemeier (925) 423-2627 (buddemeier1@llnl.gov)

Physics Today article highlights LDRD research

The recent *Physics Today* article "As weapons work slows, DOE labs keep busy with research" references three of the Laboratory's LDRD projects. The first, the Dynamic Underground Stripping Project, was led by Roger Aines (of AEED) and Robin Newmark (formerly of Global Security). The second, the Transformational Materials Initiative, was led by Bob Maxwell (of CSD). The third was by NIF's Chris Barty, on Thompson radiation extreme x-ray sources.

Contact: Roger Aines (925) 423-7184 (aines1@llnl.gov)

Business aspects of LLNL proton therapy highlighted

A September 4, 2009 article in the *San Francisco Business Times* highlights the Laboratory's proton technology, which is explained by PLS's George Caporaso (pictured at the Lab's 20-meter-long particle accelerator). TomoTherapy, of Madison, WI, has licensed the technology to treat cancer. Doctors say more patients would be treated with proton therapy if more proton therapy centers were built—currently only six proton accelerators are in use for cancer treatment domestically. These centers are too big and expensive—costing up to $200 million to build and taking up 90,000 to 130,000 square feet—for use in widespread treatment. Using LLNL technology, TomoTherapy aims to change that by creating a much smaller and cheaper machine. Compact Particle Acceleration Corporation, established by TomoTherapy to commercialize LLNL's proton therapy technology, expects to have a prototype ready by 2012 and is currently soliciting investors to finance development.

Contact: George Caporaso (925) 422-7852 (caporaso1@llnl.gov)

Scientist speaks on radio show about nuclear energy

In a KQED radio broadcast about the future of nuclear power in California, Bill Halsey (AEED) talked about the Laser Inertial Fusion Engine concept ("It's not the lowest hanging fruit, but it's the juiciest"), 4th-generation nuclear reactors ("more efficient and safer than previous designs"), and the state of California ("likely to be a follower rather than a leader on nuclear power in the near future").

Contact: Bill Halsey (925) 423-1133 (halsey1@llnl.gov)

Geoscientist talks about women in science on radio show

Motivated by the news of two female winners of the Nobel Prize in Medicine, a National Public Radio reporter visited the recent Radionuclide Migration international meeting at Washington State and talked to several female scientists presenters, including PLS's Annie Kersting, who is known for her seminal work on the colloidal transport of plutonium. Annie told the reporter that in the field of radiochemistry, there is a shortage of both women and men, and noted that DOE is investing in certain universities to try to rectify the situation. The story aired October 7 on Northwest Public Radio in Washington State.

Contact: Annie Kersting (925) 423-3338 (kersting1@llnl.gov)

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